APPENDIX J

Groundwater Contaminant Flow Transport Model Description

WORK PLAN

MATHEMATICAL MODEL OF GROUND WATER CONDITIONS

SOUTHWESTERN SALT LAKE COUNTY, UTAH

INTRODUCTION

This document provides a work plan for development of a numerical model of ground water conditions in the southwestern portion of Salt Lake County. This model is being prepared as part of the five-year joint investigations for the mine area at Kennecott's Utah Copper Division (UCD). Dames & Moore will take the lead role in developing this model, with the U.S. Geological Survey (USGS) acting under a cooperative agreement with the Utah State Health Department (USHD) and Kennecott participating in advisory and review capacities. The data base used in constructing this model will be data previously collected and assembled during Kennecott's five-year study and other data sources. Collection of additional field hydrogeological data is not planned.

PURPOSE AND OBJECTIVES

The purpose of the model is to obtain a quantitative understanding of the hydrogeology in this area, to evaluate past impacts to the ground water quality by Kennecott and others, and to provide a tool for predicting future ground water quality conditions. Specific objectives of this modeling include:

1. Organizing the hydrogeologic data into a consistent conceptual hydrogeologic model.

2. Estimating the extent of past and existing contaminant plumes.

3. Establishing past and present contaminant sources and flow pathways.

4. Simulating future conditions, specifically:

    - Extent and concentrations of contamination

    - Impact of ground water withdrawals upon contaminant migration

    - Effectiveness of remedial actions

The model area would include the area of Kennecott's five-year hydrogeologic study. The area is located in southwestern Salt Lake County, bound on the west and south by the Oquirrh and Traverse Mountains, approximately the Jordan River on the east, and 5400 South Street (on the north). The model may be extended somewhat beyond these limits if necessary to allow simulation of potential major hydrologic effects in adjacent areas.

SCOPE OF WORK

The scope of work for this project consists of the development of a mathematical model of ground water conditions calibrated to available hydrogeological and hydrochemical data. Model development will be completed in the tasks summarized below:

- Data base synthesis
- Selection of forecast scenarios
- Selection of numerical model configuration
- Selection of criteria for model calibration
- Calibration of model
- Simulation of future conditions
- Preparation of a summary report

A series of milestone reports will be prepared during the course of the study as shown on Figure 1, Schedule, and discussed herein. The tasks outlined above were selected to facilitate participation and review by Kennecott, the USGS, and other parties during the course of the project.

DATA BASE SYNTHESIS

The purpose of this task is to conceptualize the ground water system, summarize available data, and bring together the data required in subsequent tasks. Data sources utilized will include Kennecott's computer data base, Kennecott's annual data reports, internal Kennecott reports, USGS reports and files, State Engineer's reports and files, municipal records, consulting engineers reports, and other sources.

In developing the conceptual system, results of past modeling efforts in this area will be reviewed and considered. These previous models include the analog model of Hely (1971) and numerical models of the Jordan Valley prepared by the USGS (1986) and the vertical cross-section model completed by Breham (1984).

At the conclusion of this task, a document will be prepared that contains as a minimum the following information:

1. A bibliography of information sources pertinent to the model area.

2. Tabular summary of hydrologic system parameters with a listing of specific references containing information concerning those parameters in the model area.

3. A series of maps will be prepared of the model area giving:

    a. Location of wells and exploratory borings with cross-reference number.

    b. Location of significant surface features such as perennial streams, ponds, canals, dump areas, dump leaching areas, potential contaminant sources and major pumping centers.

    c. Outlines of geohydrologic units, their base elevation and thickness.

    d. Water level elevations and interpreted contours for key time periods by aquifer.

    e. Concentrations of key chemical parameters such as sulfate, chloride, total dissolved solids, and pH, and interpreted contours for key time periods by aquifer.

4. A series of geologic cross-sections in the model area.

5. A series of graphs showing changes in water levels with time for representative wells.

6. A series of graphs of key chemical parameters vs. time for representative wells.

7. Summary of projections of future ground water development and water use in the model area.

8. A concise discussion of the interpreted physical hydrogeology of the model area including number of aquifers, aquifer geometry, interconnection between aquifers, transmissivities, storage coefficients, porosities, boundary conditions, recharge (from precipitation, mountain front, streams, canals, Bingham Canyon Reservoir, the evaporation ponds, dump areas, and other major features), and discharge from subsurface outflow from the model area, evapotranspiration, and major pumping centers.

9. A concise discussion of water quality conditions in the model area including background quality of surface water and ground water, water quality of contaminant sources, and changes in surface and ground water quality over time.

These interpretations will also be shown diagrammatically and on tables and figures. These will subsequently be used in selecting calibration criteria and model design, and in preparation of model input parameters.

SELECTION OF FORECAST SCENARIOS

Since one of the primary reasons for development of the model is to forecast future aquifer conditions, it is necessary to outline conditions that will be assumed to exist and results desired from these forecasts prior to model selection. The information needed for this task includes estimates of future ground water consumption in this area, changes in land use which affect the hydrology (such as irrigation practices), and contaminant control programs either underway or proposed (such as the replacement of Kennecott's Bingham Reservoir). Potential future contaminant sources, such as leachate from landfills, will also be considered for input to the model. As output of this task, several future scenarios would be proposed representing a range of forecast conditions and control alternatives, to be modeled during subsequent tasks.

SELECTION OF NUMERICAL MODEL

Dames & Moore proposes to use its finite difference model code named TARGET, which is capable of simulating ground water flow, solute transport, dispersion and various geochemical effects upon ground water quality. Technical and mathematical descriptions of this model as well as some reviews of its use on other projects have been included as an attachment to this work plan. The purpose of this task is to select the model configuration, the initial hydrologic parameters to be used, and specific approach to calibration and forecasts. This will include selection of the model representation of:

- The aquifer in terms of number of layers and vertical grid spacing
- Horizontal grid spacing
- Boundary conditions
- Recharge/discharge conditions
- Initial assigned parameter values

As a part of this task, several preliminary model runs will be completed to help optimize execution of the model by varying grid spacings and time steps.

SELECTION OF CRITERIA FOR MODEL CALIBRATION

Based on the available data for model area, the calibration approach and model configuration, the criteria used in model calibration and verification will be selected to define minimum standard for model simulation of past and/or current hydrogeological and hydrochemical conditions.

Output from this task will consist of a document that defines the calibration criteria and provides the specific data to be calibrated against. The calibration criteria will be chosen considering the accuracy and certainty of the data and the significance of the hydrologic features to the numerical model and the needed results of the modeling effort.

MODEL CALIBRATION

The numerical model will be calibrated and verified for a series of conditions including both steady-state and transient flow. We expect that an initial (background) condition would be established for the model area by calibrating to head conditions and ground water quality conditions in a steady-state mode. Calibration/verification would be performed through model runs by matching transient water quality conditions. The key calibration will be to historic water quality changes since it appears that significant historic head changes have not occurred. The water quality constituents sulfate and TDS will be considered in the calibration since these parameters are the most indicative of Kennecott's potential contaminant sources. The criteria to be met in the calibration of the model will be defined by work completed under the task "Selection of Criteria for Model Calibration."

It is anticipated that many of the original model input parameters will need to be changed as a part of model calibration to obtain the match to measured conditions. In changing them, those parameters having the lowest degree of certainty will be changed first. All changed data will be checked for reasonableness.

Output from this work task will show the results of the model calibrations compared to observed data in a series of maps and graphs. Contour maps showing the distribution of heads and water quality data will be shown for steady-state conditions and for time periods used in calibrating to transient conditions. Where appropriate, time graphs of heads and water quality as a function of time will also be prepared.

SIMULATION OF FUTURE CONDITIONS

Forecasts of future ground water quality, contaminant migration, and head conditions will be made based upon the scenarios outlined under the task "Selection of Forecast Scenarios." These originally anticipated conditions may be modified after the calibration of the model to reflect any additional understanding of the aquifer system achieved during model calibration. These forecasts of future ground water conditions will be made based upon several scenarios of future aquifer withdrawals and man-made activities. Potential impacts of Kennecott activities and the effectiveness of alternative remedial actions upon ground water quality will be evaluated.

SUMMARY REPORT

Upon the conclusion of all modeling activities, a summary report will be prepared which consists of a main section summarizing the results of the model and appendices that detail its development, calibration and use. The report will include:

1. An executive summary

2. A compilation of all important data and references

3. A description of the conceptualized hydrogeological system

4. A discussion of site conditions as they relate to contaminant sources, ground water flow, and contaminant migration

5. A complete description of the mathematical model that includes:

   - The theoretical foundations of the model
   - All input parameters
   - Results of model calibration including maps and figures that show comparison of calculated with observed data
   - Modeled forecast conditions and results

6. A discussion of conclusions reached as a result of the modeling

7. Recommendations for future modeling work and uses of the model

USGS PARTICIPATION AND REVIEW

Kennecott has requested that the USGS assist through their cooperative program with the USHD in the development of this model through an advisory and technical review capacity. In developing the work plan, we have anticipated technical input from Kennecott and the USGS at key points during the project, generally at the conclusion of each task. At each of these points Dames & Moore will submit to Kennecott a brief progress report summarizing the pertinent information and conclusions reached and the plan for the next task. It is anticipated that these reports would be forwarded to the USGS and would serve as the basis of their review of work completed. Subsequently, Dames & Moore will meet with the USGS and Kennecott to obtain their review of the completed work, recommendations for any changes in this work, and recommendations concerning work to be completed during the next work phase. It is anticipated that any differences in opinion on technical matters between Dames & Moore, Kennecott and/or the USGS would be resolved prior to starting the next task. Any outstanding differences will be resolved by Kennecott.

PROJECT STAFFING

Mr. George Condrat will serve as Project Manager and will be responsible for overall conduct of the modeling effort. Dr. Richard Jones will be Principal Investigator and will be responsible for data synthesis, hydrologic interpretations, model development, and execution. Ms. Joanna Moreno will be responsible for the TARGET code and its numerical execution. Mr. John Brown will complete much of the data collection and summary needs of the work. Mr. Condrat, Dr. Jones and Mr. Brown have all been actively involved in the ongoing Kennecott Hydrogeologic Study and are familiar with the study area. Ms. Moreno has performed a large number of similar modeling projects and was a principal developer of the TARGET code. Additional personnel will be drawn from our Salt Lake staff for technical, illustration, and clerical needs as required.

PROJECT SCHEDULE AND COST

The proposed schedule for completion of this work is provided on Figure 1. We have set the duration of the schedule for 10 months, which should allow adequate time for review and advisory inputs to the project.

The estimated cost for completion of this work is $125,000. A detailed breakdown of the estimated charges is provided in Table 1.

COST ESTIMATES

KENNECOTT GROUND WATER MODEL

Task	Estimated Cost
Data Base Synthesis	$ 20,000
Selection of Forecast Scenarios	5,000
Selection of Numerical Model Configuration	10,000
Selection of Calibration Criteria	5,000
Calibration of Model	50,000
Simulation of Future Conditions	15,000
Summary Report	15,000
Project Review	5,000
Total	$125,000

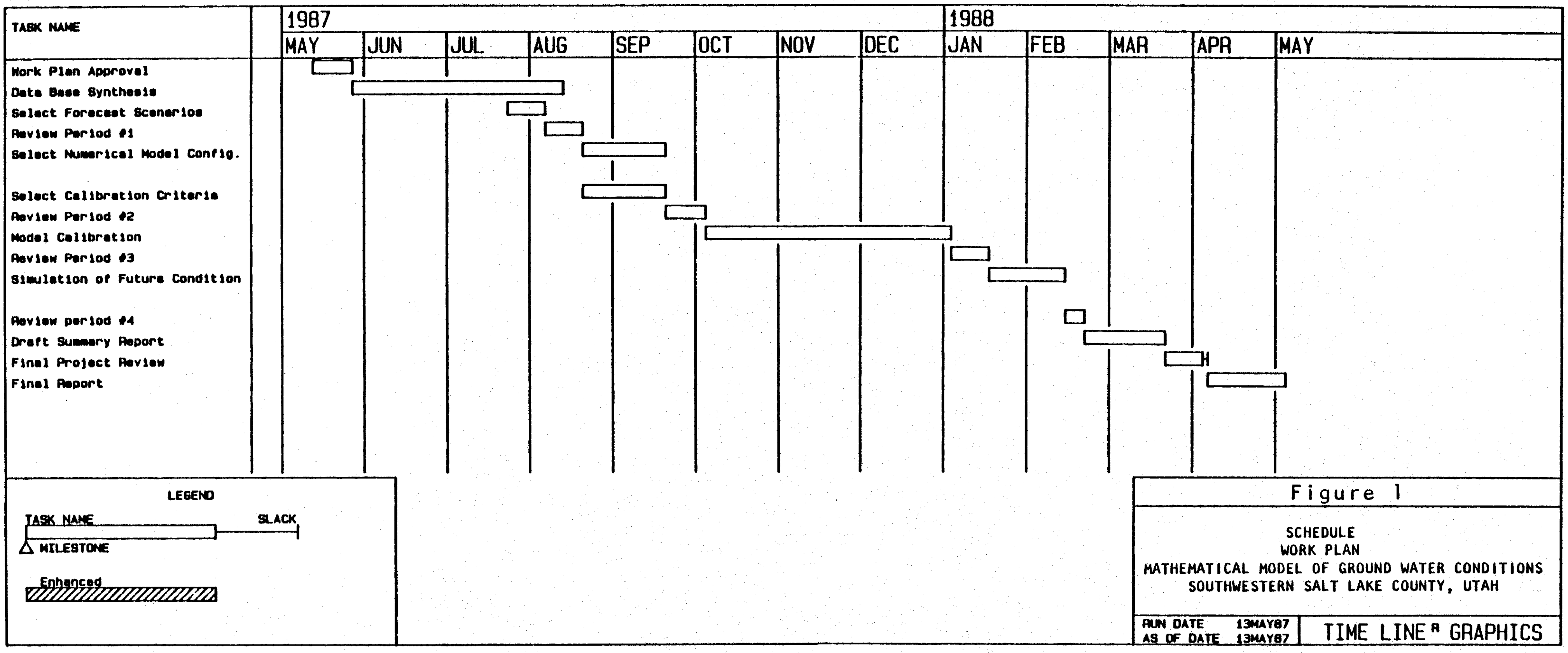

Figure 1

SCHEDULE
WORK PLAN
MATHEMATICAL MODEL OF GROUND WATER CONDITIONS
SOUTHWESTERN SALT LAKE COUNTY, UTAH

TARGET

Dames & Moore Mathematical Model Of Ground-Water Flow And Solute Transport: Summary Of Background To Variably-Saturated And Density-Coupled Models

TABLE OF CONTENTS

1.0 INTRODUCTION

This appendix summarizes the physical and chemical hypotheses, mathematical formulation, and numerical framework of a numerical model of ground-water flow and chemical-species transport in variably-saturated porous media. The numerical model, developed by Dames & Moore over the past 5 years, is known as TARGET (Transient Analyzer of Reacting Ground Water and Effluent Transport). The purpose of this document is to provide a general description of the methodology and assumptions employed in the model.

Documents covering details of the mathematical formulation, model input data structure and definitions, and validation cases covering the range of model applicability, are available separately. Due to similarity in approach, this appendix relates to three of the series of five models in the TARGET family; namely TARGET_2DU (two-dimensional, vertical cross section, variably-saturated), TARGET_3DU (three-dimensional, variably-saturated), and TARGET_3DS (three-dimensional, fully saturated).

The state-of-the-art of mathematical models for predicting fluid dynamics and associated mass transport in variably saturated porous media has advanced considerably within the past few years. The literature describing these advances is vast; it has been reviewed by several authors including Narasimhan and Witherspoon (1977), Lappala (1980) and Heijde, et al. (1985). Comprehensive reviews of ground-water numerical modeling techniques are provided by Remson, et al. (1971), Pinder and Gray (1977), and Mercer and Faust (1981). The model presented in the following pages falls into the category of integrated finite-difference procedures which solve the density-coupled flow and reactive mass transport equations in variably-saturated porous media by employing a sophisticated hybrid differencing scheme. Details of the mathematical formulation of the model are presented in Dames & Moore (1985a and b). Applications of the model have been reported by Highland, et al. (1983) and Sharma, et al. (1983) among others.

The TARGET model capabilities include accommodation of the following site features:

- Physical mechanisms which influence hydrodynamics:
  - Regional or local recharge or discharge
  - Hydraulic and density induced pressure gradients
  - Compressibility of the matrix and water
- Variable saturation
- Material-property variations
- Boundary conditions of all types:
  - Specified head boundaries
  - Specified flux boundaries
  - Mixed boundary conditions
- Man-made features:
  - Injection or extraction wells
  - Waste disposal facilities
  - Pollution-abatement measures

° Mass transport mechanisms:

- Advection
- Dispersion
- Density effects
- Viscosity effects
- Sorption and chemical reactions.

Models of the TARGET family have been applied in more than 80 projects to a range of water management and contaminant control problems including: dewatering of multiple aquifers during operation of an Australian strip mine, simulation of alternate remedial measures at five Superfund sites, and prediction of containment and extraction of light hydrocarbons and dense mine wastes. During the course of these applications, the model approach and predictions have been reviewed and approved by many regulatory agencies including the U.S. Geological Survey and U.S. Environmental Protection Agency. In addition, a satisfactory peer review of the model formulation by Professor Allan Freeze was solicited by Dames & Moore. These review opinions, as well as publications and model validation cases, provide the basis for background substantiation of model predictions.

2.0 PHYSICAL MECHANISMS AND CHEMICAL PROCESSES

The purpose of this section is to summarize the major assumptions used in developing the physical and chemical hypotheses embedded in the model.

Ground-Water Flow

The flow mechanisms incorporated in the model are unsaturated pore-pressure gradients, saturated pressure head gradients, gravity-induced and density-induced pressure gradients, as well as changes in storage due both to compressibility of the ground water and the matrix and water-table fluctuations. Assumptions made in the development of the hydrodynamic equations for saturated-unsaturated flow presented in Section 3.0 are:

- The porous medium is deformable, but not consolidating.
- Ground water is compressible, but density changes due to compression are neglected.
- In unsaturated regions, pressure gradients in the air are negligible and air pressure is equal to atmospheric pressure.
- An empirical expression (Darcy's law) can be used to relate macroscopic ground-water velocity to the gradient of pore-fluid pressure.
- Changes in storage due to changes in pressure are the result of both the elastic properties of the aquifer and ground water, and drainage from pores.
- The principal directions of the hydraulic conductivity tensor are aligned with the cartesian coordinate system adopted in the model.
- Evaporation from the water table may be neglected.

In order to completely describe the physical processes occurring in variably saturated soils, auxiliary relationships describing the variation of hydraulic conductivity, $Kr(\psi)$, and degree of saturation, $Sr(\psi)$, with negative pore pressures must be defined. In general, the relationships may only be realistically obtained through laboratory measurements of the soil types of interest. However, an S-shaped curve may be expected for most soil types (see

Figures 2.1 and 2.2) and several authors have developed derivations for $Kr(\psi)$ based on the corresponding $Sr(\psi)$ relationship (e.g., Jackson, et al., 1965 and Mualem, 1976). The following forms of relationships fit most data sets and are used in the model:

$$Sr = \frac{\theta_r}{\theta_s} + \left(1 - \frac{\theta_r}{\theta_s}\right) \left\{ 1 + (a_{0s} |\psi|)^{a_{1s}} \right\}^{-a_{2s}} \qquad ; - \infty < \psi < 0$$

$$Sr = 1 \qquad ; \quad \psi > 0 \qquad (2\text{-}1)$$

$$Kr = Kr_{min} + (1 - Kr_{min}) \left\{ 1 + (a_{0k} |\psi|)^{a_{1k}} \right\}^{-a_{2k}} \qquad ; - \infty < \psi < 0$$

$$Kr = 1 \qquad ; \quad \psi > 0 \qquad (2\text{-}2)$$

where:

a_{0s}, a_{1s}, a_{2s} = coefficients in Sr relationship
a_{0k}, a_{1k}, a_{2k} = coefficients in Kr relationship
Kr = relative hydraulic conductivity [-]
Kr_{min} = minimum relative hydraulic conductivity for dry conditions
θr = residual moisture content [-]
θs = saturated moisture content [-]
Sr = degree of saturation [-]

Solute Transport

The model described in this appendix has been designed to simulate the movement of dissolved constituents of similar or different density and viscosity than ground water, in variably saturated soil and rock. The transport mechanisms incorporated in the model are advection, mechanical dispersion, molecular diffusion, and equilibrium sorption. Density driven flows are included, but thermally driven flows are excluded from the solute transport

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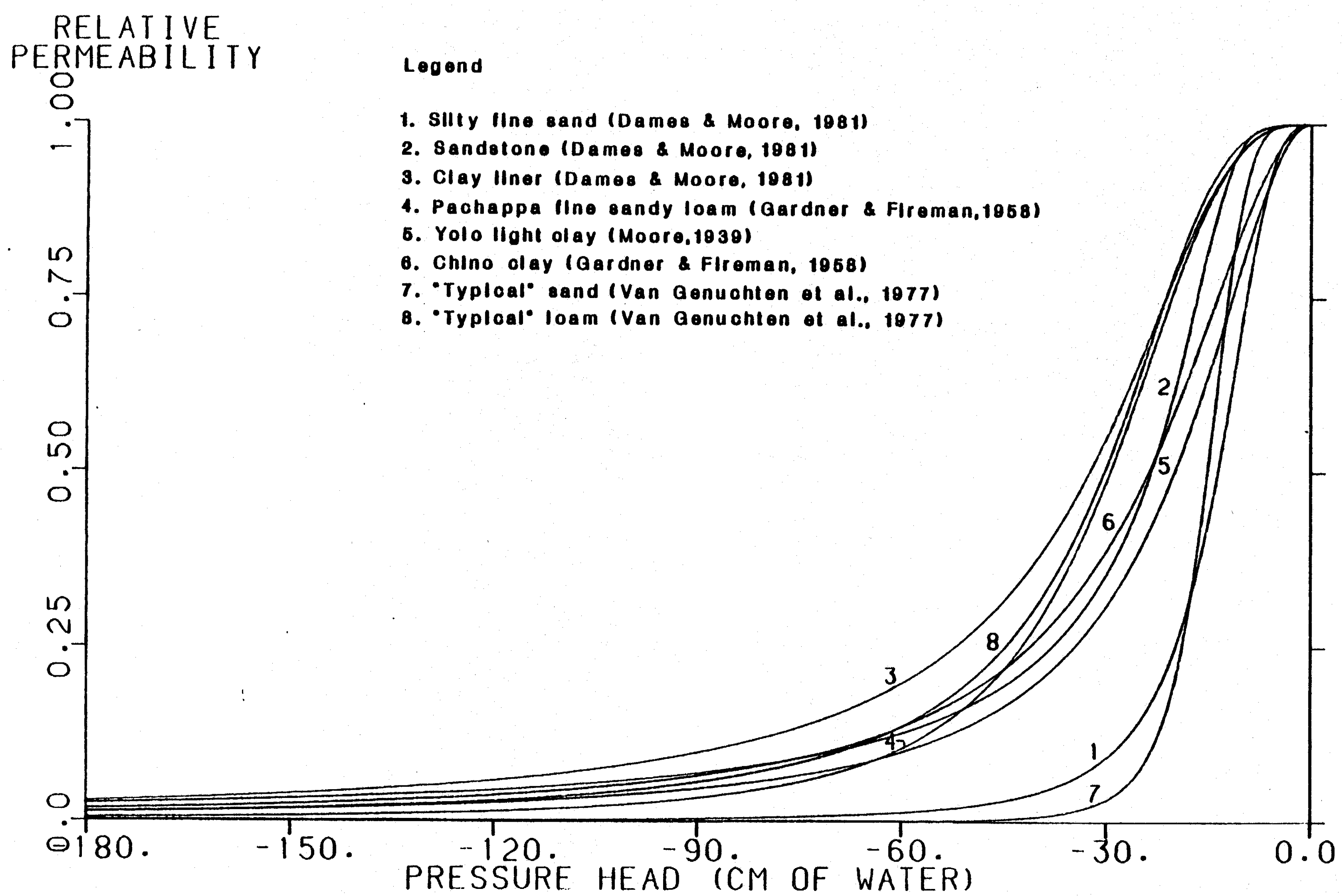
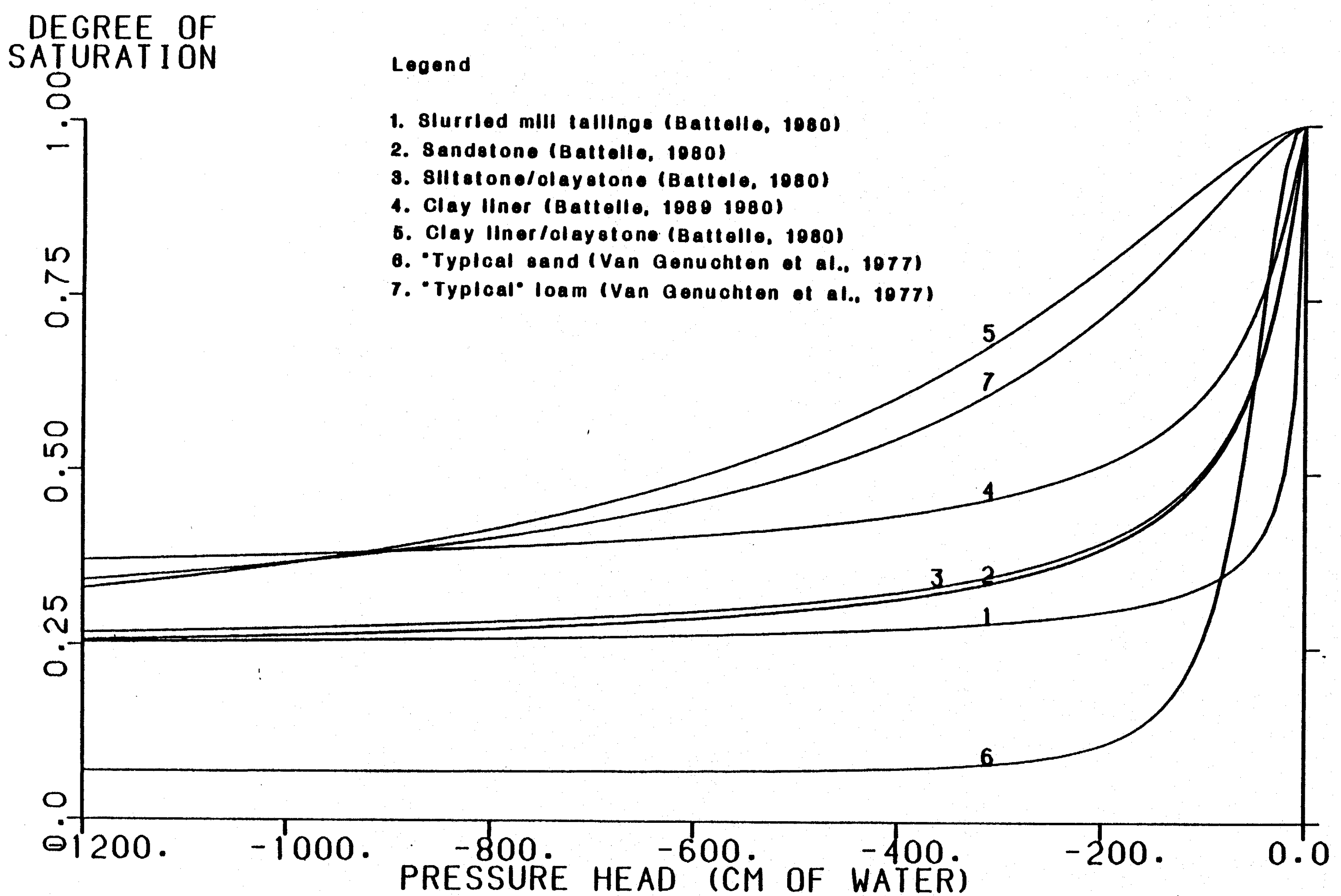


Relationship Between Relative Permeability And Pressure Head For Various Soils

Fig 2.1



Relationship Between Degree Of Saturation And Pressure Head For Various Soils

Figure 2.2

mechanisms. Density differences of about 1 percent are known to significantly influence subsurface fluid movement (Mackay, et al., 1985). The local density and viscosity are assumed to be linearly related to the predicted solute concentration in the model. Typically, linear or near-linear relationships (e.g., Kendall-Monroe equation for viscosity of miscible liquid solutions, Arrhenius equation for viscosity of emulsions) are appropriate for organic solutions (Perry and Chilton, 1973), as well as for metals and total dissolved solids (Dames & Moore, 1983).

Dispersion of solutes is caused by both molecular diffusion (dependent on local concentration gradients) and mechanical dispersion (due to tortuous solute flow paths on a microscopic level). Because microscopic measurements are not practical on a field scale, empirical relationships form the basis for describing these physical phenomena. TARGET uses the most widely accepted relationship for dispersion (Huyakorn and Pinder, 1982):

$$D_{ij} = D_T|U|\delta_{ij} + (D_L - D_T)\frac{U_i U_j}{|U|} + D_d\tau \qquad (2\text{-}3)$$

where:

D_d = molecular diffusion coefficient $[L^2/T]$
D_{ij} = dispersion coefficient tensor $[L^2/T]$
D_T = transverse dispersivity [L]
D_L = longitudinal dispersivity [L]
U_i = i-direction particle velocity component [L/T]
δ_{ij} = Kronecker delta [-]
τ = tortuosity [-]

In characterizing the mobility and attenuation of solutes, it is essential to quantify the geochemical mechanisms which influence or control the chemical interactions between subsurface media and the fluids contained in them.

Predominant among such mechanisms are mechanical filtration, cation exchange, buffering of pH, chemical precipitation due to reactions with the solid matrix as well as with interstitial water, hydrolysis, and oxidation-reduction reactions. The factors which make such a quantification difficult are the kinetic or non-equilibrium nature of certain reactions, competition between mechanisms and chemical species, and multi-layer adsorption. While a number of adsorption models have been proposed in the literature (e.g., Cameron and Klute, 1977; Valocchi, 1984; Goltz and Roberts, 1984), the best approach for a particular study rests on the solute(s) and geochemical environment involved. The version of TARGET described here uses a linear adsorption isotherm:

$$m_{J,s} = Kd\ C_J \tag{2-4}$$

where:

$m_{J,s}$ = mass concentration in the solid phase [M/M]
C_J = volumetric concentration in the liquid phase [L^3/M]
Kd = adsorption distribution coefficient [L^3/M]

which incorporates assumptions that equilibrium is immediately established (or at least reactions occur much faster than ground-water flow) between adsorption and desorption, and adsorption is reversible. Alternate adsorption isotherms may be readily incorporated in the model if appropriate. Evidence suggests that linear adsorption isotherms are representative of organic contaminant behavior for concentrations up to the aqueous solubility (Chiou, et al., 1979), but that adsorption of metal contaminants may be strongly dependent on the local pH (Dames & Moore, 1981).

3.0 MATHEMATICAL FORMULATION

3.1 Governing Equations

Three basic equations govern flow and solute transport in variably saturated porous media. These are:

- The equation of conservation of ground-water flow (i.e., mass conservation of ground water);
- Darcy's law; and
- The equation of conservation of chemical product in solution in ground water (solute); also referred to as the equation of mass transfer.

The mathematical derivation below shows how these three basic equations are transformed into two relationships of the primary variables:

ψ (pressure head) and,

m_J (mass concentration of chemical product J).

A three-dimensional cartesian system of coordinates is used in the following derivations and, consequently, the remainder of this appendix is applicable to both three-dimensional and two-dimensional, cross section (profile) situations.

1. Conservation of Ground-Water Flow

The fundamental three-dimensional mass conservation equation for variably saturated porous media is expressed as follows (Bear, 1979, p. 213):

$$\underbrace{\frac{\partial}{\partial t}\left\{nSr\rho\right\}}_{\text{storage}} + \underbrace{\frac{\partial}{\partial x_i}\left\{nSr\rho U_i\right\}}_{\text{in/out flow}} = \underbrace{\dot{m}'''}_{\text{source/sink}} \tag{3-1}$$

where:

$\dot{m}'''$ = specific mass source rate [M/TL^3]
n = porosity [-]
Sr = degree of saturation [-]
t = time [T]
U_i = i-direction particle velocity [L/T]
x_i = i-direction coordinate [L]
ρ = density [M/L^3]

2. Darcy's Law

The generalized form of Darcy's law in anisotropic porous media can be expressed as follows (Bear, 1979, p. 64):

$$\underbrace{nSrU_i}_{\text{Darcy velocity}} = -Kr\frac{k_{ij}}{\mu}\underbrace{\left\{\frac{\partial p}{\partial x_j} + \rho g\frac{\partial Z}{\partial x_j}\right\}}_{\text{total pressure gradient}} \tag{3-2}$$

where:

g = gravitational acceleration [L/T^2]
k_{ij} = intrinsic conductivity tensor component [L^2]
Kr = relative conductivity [-]
p = pressure [M/LT^2]
Z = vertical axis [L]
μ = viscosity [M/LT]

3. Conservation of Chemical Product in Solution

The fundamental three-dimensional conservation equation for a chemical product in solution in ground water is expressed as (Bear, 1979, p. 239):

$$\underbrace{\frac{\partial}{\partial t}\left\{ nSr\rho m_J \right\}}_{\substack{\text{storage in} \\ \text{mobile phase}}} + \underbrace{\frac{\partial}{\partial t}\left\{ (1-n)\rho_s\, m_{J,s} \right\}}_{\substack{\text{storage in} \\ \text{immobile phase}}} + \underbrace{\frac{\partial}{\partial x_i}\left\{ nSr\rho U_i m_J \right\}}_{\text{advection}} = \underbrace{\frac{\partial}{\partial x_i}\left\{ nSr\rho D_{ij}\frac{\partial m_J}{\partial x_j} \right\}}_{\text{dispersion}} + \underbrace{\dot{m}''' M_J}_{\substack{\text{source/} \\ \text{sink}}} \tag{3-3}$$

where:

D_{ij} = dispersion coefficient tensor $[L^2/T]$
m_J = mass concentration of chemical product of J in liquid phase [M/M]
$m_{J,s}$ = mass concentration of chemical product of J in solid phase [M/M]
M_J = source mass concentration of chemical product of J [M/M]
ρ_s = soil bulk density $[M/L^3]$.

Upon introducing Darcy's law (3-2) into the equation of mass conservation (3-1) and transforming the time dependent term through the use of the concept of specific storage, the mass conservation equation may be expressed as a single equation of the dependent variable, ψ (pressure head):

$$RSrSc\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial x_i}\left\{ RKrK_{ij}M\left[\frac{\partial\psi}{\partial x_j} + R\frac{\partial Z}{\partial x_j}\right] \right\} - Rn\frac{\partial Sr}{\partial t} - nSr\frac{\partial R}{\partial t} + \frac{\dot{m}'''}{\rho_o} \tag{3-4}$$

where:

Pressure head $\psi \equiv \dfrac{p}{\rho_o g}$

Density ratio $R \equiv \dfrac{\rho(m_J)}{\rho_o}$

Viscosity ratio $M \equiv \dfrac{\mu_o}{\mu(m_J)}$

Hydraulic conductivity $K_{ij} \equiv \dfrac{k_{ij}\rho_o g}{\mu_o}$

Sc = specific storage coefficient [1/L]
ρ_o = reference density [M/L^3]
μ_o = reference viscosity [M/LT]

The fundamental form of the mass transfer equation (3-3) requires additional relationships to completely define the problem of transport of a chemical product in variably saturated porous media:

° Relationship to link the concentration of the chemical product in the solid matrix to that in the ground water; and

° Relationship to link the coefficients of the dispersion tensor to the longitudinal and transverse dispersivities.

The solid/fluid interaction is assumed to be represented by a so-called linear isotherm (2-4). Under this assumption the matrix concentration, M_{Js}, can be rewritten as:

$$m_{J,s} = \rho Kd\, m_J \tag{3-5}$$

Upon introducing the equation for solid/fluid interaction (3-5) and the relationship for the diffusion coefficients (2-3) into the fundamental mass transfer equation (3-3), the mass transfer equation may be expressed as:

$$\begin{aligned} nSrR \frac{\partial m_J}{\partial t} + R_b R \rho_o Kd \frac{\partial m_J}{\partial t} + nRSrU_i \frac{\partial m_J}{\partial x_i} = \\ \frac{\partial}{\partial x_i} \left\{ RnSrD_{ij} \frac{\partial m_J}{\partial x_i} \right\} + \frac{\dot{m}'''}{\rho_o} [M_J - m_J] \\ - m_J \left\{ \frac{\partial}{\partial t} (nRSr) + \frac{\partial}{\partial x_i} (nSrU_i) - \frac{\dot{m}'''}{\rho_o} \right\} \end{aligned} \tag{3-6}$$

where:

$$R_b = \frac{\rho_b}{\rho_o} = [1-n] \frac{\rho_s}{\rho}$$

ρ_b = soil (grain) density $[M/L^3]$

3.2 Guess and Correct Algorithm

Prior to the transformation of the partial differential equations into their finite-difference form and implementation in the numerical model, equations (3-4) and (3-6) are modified using a guess and correct (or predictor/corrector) algorithm. This technique was implemented because of its numerical advantages primarily when solving for variables such as pressure head, with which it is common to encounter relatively large mean values and small but highly significant gradients.

The basis of this algorithm consists in substitution for the dependent variable in the partial differential equations by the sum of a guessed value and a correction to be applied to the guessed value. The terms are then grouped and the resulting equation expressed in terms of the correction with a distributed source representing the accuracy of the guess value. The converged solution for the dependent variable is thus zero throughout the calculation domain.

3.3 Initial Conditions

Initial distribution of the dependent variables (or in the guess and correct nomenclature initial guessed value) of the pressure head ψ, and of the mass concentrations of the chemical product m_J are necessary. These can be derived from observed or postulated field conditions or through the calculation of steady-state distributions with appropriate boundary conditions. Often, partially saturated initial conditions are available, from field data, in the form of the moisture content distribution. It is of particular importance to the correct prediction of transient phenomena to obtain good initial conditions; i.e., flow field and concentration distributions which obey the conservation principles. Failing to follow these requirements, unwanted pressure redistribution and mass transport may take place in the early stages of a transient calculation. In other words, the initial conditions of a transient calculation are usually the result of a preliminary steady-state or transient calculation.

3.4 Boundary Conditions

Boundary conditions for the primary variables are required to complete the problem definition.

The various types of boundary conditions encountered in flow and solute transport through porous media are:

1. Prescribed Boundary Values - The pressure head or the concentrations are assigned a prescribed value along the entire boundary or sections thereof. This type of boundary condition is also called a Dirichlet boundary condition.

2. Prescribed Boundary Flux - On a boundary of this type, the flux of ground water or chemical product perpendicular to the boundary is prescribed. A special case of this type of boundary is the impervious boundary where the flux is zero. This type of boundary condition is also called a Neumann boundary condition.

Other types of boundary conditions, such as Cauchy, also called mixed boundary conditions, can be represented by combinations of the above two types. Although seepage faces can be represented by the above types of boundary conditions, the correct point of exit has, generally, to be approached through a series of trial-and-error steady-state solutions. All of the boundary condition values may further vary with time.

3.5 Internal Sources and Sinks

Often, practical problems require that man-made or natural features such as wells, rivers, lakes, ponds, infiltration, or evaporation be represented. This is generally achieved by the use of internal sink or source terms, or, by the use of prescribed values within the calculation domain as opposed to prescribed values on the boundary of the calculation domain. Sources and sinks may arbitrarily vary with time.

4.0 NUMERICAL METHODS

The numerical calculation procedures employed to solve the equation set described in Section 3.0 is of the integrated finite-difference (IFD) variety. A grid system consisting of rectangular cells of arbitrary aspect ratio, with grid nodes located at the geometrical center of each cell, serves as the basis for the derivation of the discretized (i.e., finite-difference) equations. These latter are obtained by intergrating the appropriate differential equations over each of the cells in the calculation domain. For this integration, the dependent variables are presumed to vary linearly between adjacent grid nodes. This procedure transforms the partial differential equations into two sets of algebraic linearized equations, one of the calculation of pressure head, ψ , and the other for the calculation of mass concentrations, m_J. In the case of dense chemical products, these two sets are coupled through terms representing gravitationally induced fluid motion. Because of this coupling and because of the nonlinear nature of the pressure head equation, an iterative

Alternating Direction Implicit (ADI) algorithm is used in the solution of the algebraic set of equations. Under-or over-relaxation of the iterative scheme is permitted to damp or accelerate the convergence rate of the solution.

Indiscriminate use of the finite difference discretization technique for the first and second spatial derivatives can lead to unstable and even to physically meaningless solutions when the problem is advection dominated. This may occur when the magnitude of the cell Peclet number is greater than 1. In the present model, such difficulties are overcome by the use of a hybrid differencing scheme in which upstream, downstream or central differencing schemes are employed depending on the local Peclet number and direction of flow.

Particular care is also taken with the evaluation of the local degree of saturation both due to the non-linearity of the Sr relationship and due to the close link between degree of saturation and relative hydraulic conductivity. Because the Sr (ψ) relationship is strongly non-linear the average degree of saturation of a cell is calculated on the basis of an assumed linear variation of pressure head between nodes along the vertical axis, rather than as a function solely of the pressure at the node. In addition, the formulation of the time-dependent term $\partial Sr/\partial t$ in finite difference form requires particular care as:

- It is a strongly non-linear term, highly sensitive to changes in pressure head; and
- It is the dominant term controlling changes of storage in partially saturated cells.

5.0 SOLUTION TECHNIQUES

5.1 Iterative Method

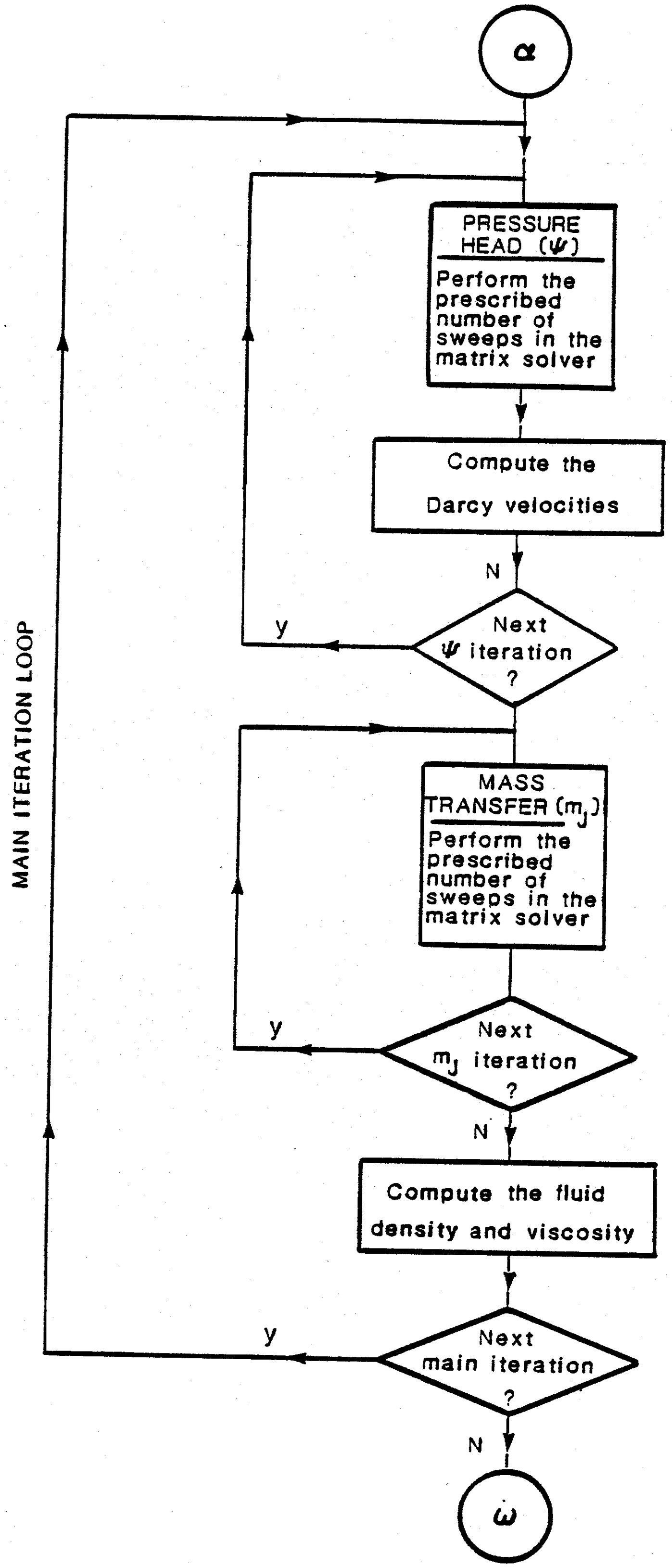
Since the pressure head equation is non-linear and since density and viscosity effects create a strong coupling between the pressure head and the mass transfer equations, an iterative solution method is required.

The iteration scheme used in TARGET is composed of three levels of iteration. These are also illustrated in Figure 5.1:

1. The main iteration loop, over the solution of both the pressure head and mass concentration equations. The objective of this loop is to account for the density and viscosity coupling effects. This loop need not be executed more than once in noncoupled problems, i.e., when the chemical product in solution in ground water has the same density and viscosity as the ground water.

2. The secondary iteration loop over the solution of the equations of pressure head and mass concentration individually. The objective of this loop is to account for the non-linear terms such as relative conductivity and degree of saturation. This loop need not be executed more than once for linear equations such as the mass transfer equation.

3. The innermost iteration loop is the matrix solution loop. The objective of this loop is to obtain a good solution for a given set of coefficients.



ITERATION SCHEME

Dames & Moore

Figure 5.1

The convergence of these various loops is tested to establish when a good solution is obtained. Experience has shown that a limited number of sweeps produce satisfactory results, the innermost loop is not tested against a particular convergence criterion and is always executed a predetermined number of times.

The secondary iteration loops are converged when the source terms of the correction equation are converging towards zero everywhere. These iteration loops are terminated when either the number of iterations exceeds a prescribed maximum number of iterations or when a tolerance criterion is met. Similarly, the main iteration loop is converged when the coupling effects have been completely transmitted between the equations of pressure head and of mass concentration.

5.2 Matrix Solution Algorithm

The solution algorithm implemented in TARGET is somewhat different in two- and three-dimensional problems. In both cases, it is based on a ADI (Alternating Direction Implicit) algorithm which in two-dimensional problems, is implemented as a line-by-line, column-by-column solution sequence of the resulting three-diagonal matrix. In three-dimensional problems, the same alternating direction scheme is used, but all planes are solved for simultaneously, which results in the solution of a five-diagonal matrix.

Taking the two-dimensional solution algorithm as an example, a complete execution of the solver is composed of a line-by-line, followed by a column-by-column solution. Each solution sweep is composed of the following steps:

- Assemble the three-dimensional matrix through suitable combination of terms.
- Apply a forward elimination, backward substitution algorithm to the resulting matrix.
- Repeat sequence an even number of times to achieve a complete solution.

5.3 Relaxation

In the guess and correct formulation, the dependent variable is a correction which has to be added to the previous value of the primary variables itself. A fully converged solution is obtained when the correction is everywhere identical to zero. Due to the non-linear nature of the coefficients, the convergence rate can show strong variations from one problem to another. In some cases, the correction starts at a high value and decreases very slowly without sign changes, while in the other cases, it may show an oscillatory pattern. In order to accelerate or damp the convergence rate, the correction is multiplied by a relaxation factor before being added to the primary variables.

Density coupled problems are of very unstable nature as the fluid densities calculated after the mass transport equation has been solved result in a substantial contribution in the pressure head equation. In order to stabilize this effect, an additional relaxation factor has been introduced on the density term itself. This approach has enabled simulation of otherwise intractable problems.

6.0 VALIDATION CASES

A selection of three validation cases are illustrated on the following pages. They have been chosen to illustrate a range of model features as well as a variety of types of validation:

- Case 3 - Comparison with analytical solution for one-dimensional transport problem.
- Case 4 - Comparison with laboratory data for two-dimensional falling water table problem.
- Case 7 - Comparison with USGS ground-water model for practical application in a mine pit backfilling investigation.

CASE 3: TARGET_2DU VALIDATION - COMPARISON WITH ANALYTICAL SOLUTION

One-Dimensional Transport
Generated April 1985

Objective: To compare the results of modeled contaminant transport in one dimension with the exact solution obtained analytically.

Description: The situation is one of uniform flow in one dimension where the specific discharge is constant along the flow axis. At some point in time, a contaminant or tracer of constant concentration is introduced into the system. The distribution of this concentration along the direction of the flow is investigated.

Specification: The initial and boundary conditions are:

if x = distance along the direction of flow;
for time ≤ 0, tracer concentration, $C = 0$ at $x = 0$
for time ≥ 0, $C = C_o$, at $x = 0$
velocity, $u = 1$ ft/day
porosity, $n = 1$

The exact analytical solution to this problem (Freeze and Cherry, 1979) is:

$$\frac{C}{C_o} = \frac{1}{2}\left[\operatorname{erfc}\left\{\frac{x-ut}{2\sqrt{Dt}}\right\} + \exp\left(\frac{ux}{D}\right)\operatorname{erfc}\left\{\frac{x+ut}{2\sqrt{Dt}}\right\}\right]$$

The finite-difference grid consists of 100 cells 10 feet long to simulate the 1000-foot-long medium being modeled.

Two cases are modeled. In the first, the longitudinal dispersivity, $D_L = 10$ feet and the Peclet number, $Pe = 2$. In the second case, $D_L = 100$ feet and $Pe = 0.2$.

Results: The results of the modeled concentrations at various times are plotted in Figures 3-1 and 3-2. The y-axis represents relative concentration (C/C_o) and the x-axis represents a quantity which is a function of distance. This representation is convenient since it allows the exact solution of concentration distribution at any time to fall on the same curve. This exact solution is the curve drawn in each figure.

The analytical solution presented by Bear (1979) is an equation containing only the first item in the above equation. A similar solution has been presented by Freeze and Cherry (1979; see above) which includes a second term in the equation. Freeze, however, indicates that the second term is negligible under certain conditions, but does not give sufficient information with which to evaluate in the general case when the term is negligible. The analytical solution presented in Figures 3-1 and 3-2 does contain the assumption that the second term is negligible.

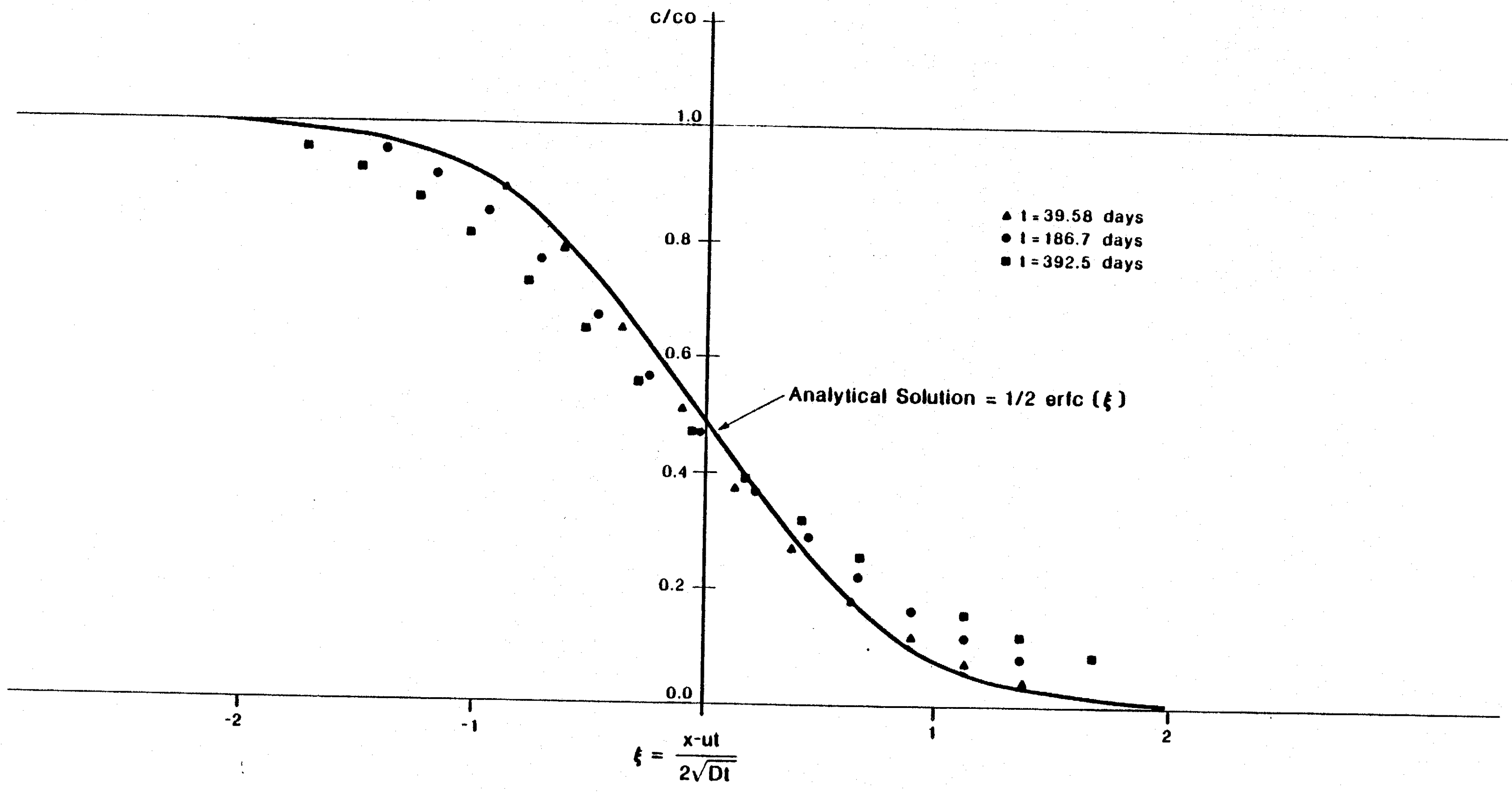
Discussion: The results of the modeled concentration distributions compare favorably with the exact solution. The fact that the $C/C_0 = 0.5$ point is not predicted to lie exactly on the x-axis where $x = 0$ indicates that the modeled location of the moving concentration "front" is slightly behind the actual location. Since the calculated difference between mass inflow and outflow was very small, the cause of this discrepancy is probably an asymmetrical calculation of the concentration rather than a loss of solute.

The results shown in Figure 3-2 are a better match to the analytical solution than those in Figure 3-1. The cell Peclet number, which is the ratio between convective and diffusive fluxes, is lower in Figure 3-2. This indicates that diffusion is the more controlling mechanism for the second figure. It is expected that a more dominant molecular diffusion action will result in predictions which more closely follow the exact analytical solution.

References:

Bear, J. Hydraulics of Groundwater, McGraw-Hill Book Company, 1979, pp. 264-265.

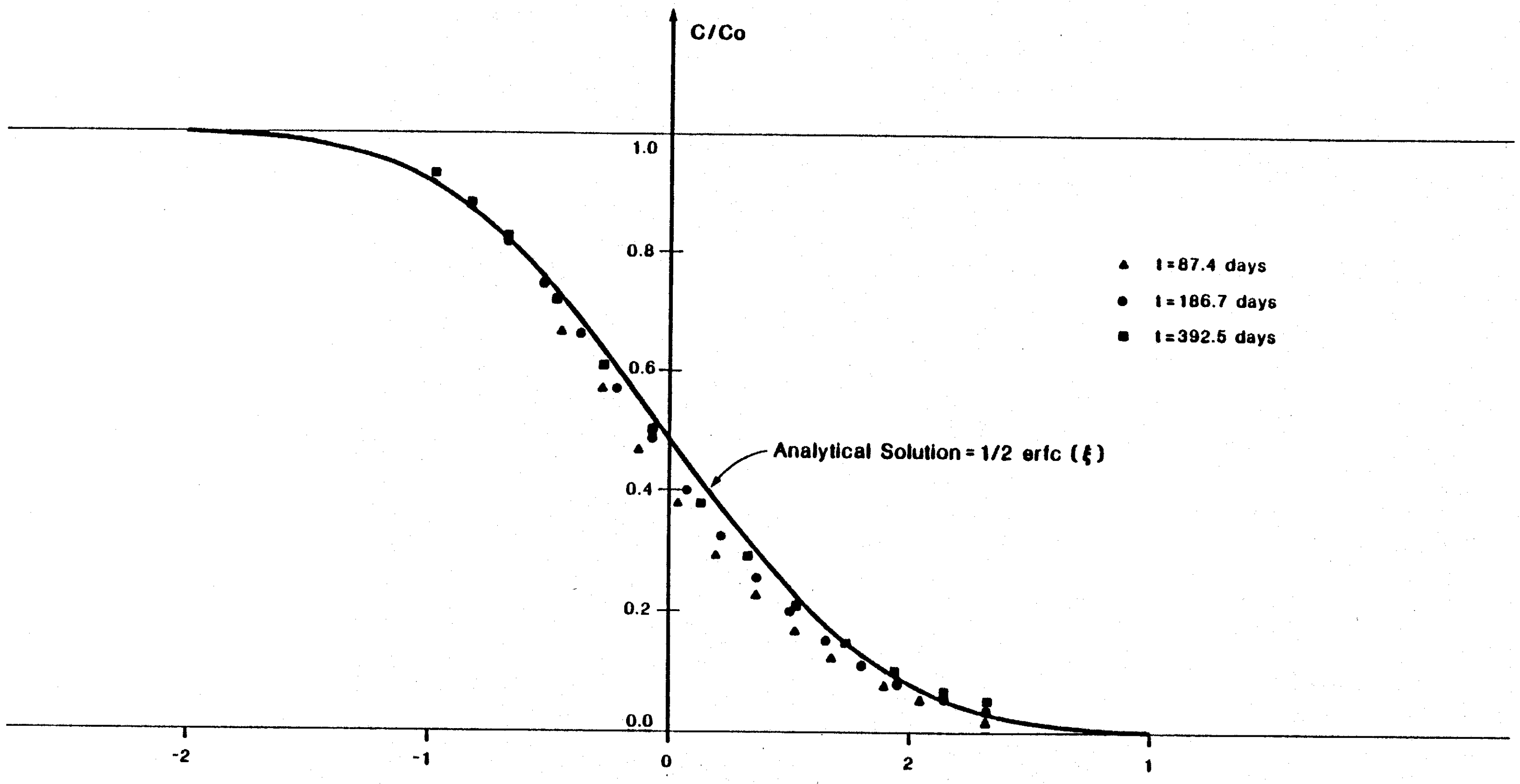
Freeze, R.A. and J.A. Cherry. Groundwater, Prentice Hall, Inc., 1979, pp. 388-393.



Modeled vs Analytical Solution

Pe = 2.0

Dames & Moore



$$\xi = \frac{X - ut}{2\sqrt{Dt}}$$

Modeled vs Analytical Solution

Pe = 0.2

Dames & Moore

Figure 3-2

CASE 4: TARGET_2DU VALIDATION - COMPARISON WITH LABORATORY DATA

Sandbox Experiment
Generated January 1983

Objective: To compare the results of the TARGET model, used to simulate transient drainage from a sandbox which was initially uniformly saturated, with laboratory data obtained in a physical experiment. The contour of zero pressure head along the length of the sandbox is plotted for various elapsed times, along with the experimentally obtained data. The primary model feature validated in this comparison is drainage from pores, i.e., transition from saturated to unsaturated conditions.

Description: The situation under investigation is the falling water table problem. A rectangular volume of sand representing a uniform aquifer is initially saturated with a horizontal zero pressure head contour at a certain height. At one end of the sandbox, water is allowed to drain while the other end is recharged. The movement of the zero pressure head contour as it seeks a new equilibrium is investigated.

Specification: The porous medium was a fine sand packed homogeneously in a box with an impervious base and sides. The situation is represented in Figure 4-1. The experimental data were gathered as described by Vachaud et al. (1971, 1975).

During the experiment, the cumulative outflow volume was controlled continuously. Recharge at the opposite end of the box was controlled so as to maintain the height of the saturated level constant at this boundary. The hydraulic conductivity-water content-water pressure head data obtained experimentally are shown in Figure 4-2. The equations used in TARGET to describe these relationships are plotted and fitted to the measured data points in this figure.

The model simulation utilized a finite-difference grid with 32 cells in the horizontal direction and 31 cells in the vertical direction. The cells ranged in size from 1 cm by 1 cm to 24 cm by 16 cm with the smaller cells concentrated in the area of drainage and shifting pressure head.

Other parameters supplied to the model include the following:

x-direction hydraulic conductivity, Kx	=	0.011 cm/sec
z-direction hydraulic conductivity, Kz	=	0.011 cm/sec
storativity, S	=	4.9 E-5
porosity, n	=	0.3

Results: The model prediction of the zero value contour of pressure head at various times is plotted in Figures 4-3 through 4-6. The experimentally obtained data for the same contour are also presented in these figures. As can be seen, the modeled results are in good agreement with the laboratory data.

Discussion: The results at four instants in time are presented in the figures. At the earliest instance, the model shows a slightly lower water table than the measured values, with the largest discrepancy at the area of steepest pressure head gradient. By the time of the next displayed instance, the two sets of data are nearly identical, and this agreement remains in the following displayed instances.

References:

Vachaud, G.M., M. Vauclin, J.L. Thony, and D. Khanji (1971). Etude Experimentale du Drainage de la Recharge des Nappes a Surface Libre dans un Modele Bidimensionel. Laboratoire de Mechanique des Fluides, Universite Scientifique et Medicale de Grenoble, Cedex, 53, 38 - Grenoble-Gare, France.

Vauclin, M., G.M. Vachaud, and D. Khanji (1975). Two-Dimensional Numerical Analysis of Transient Water Transfer in Saturated-Unsaturated Soils. Institut de Mecanique, Universite Scientifique et Medicale de Grenoble, B.P. 53 - F. 38041 - Grenoble-Cedex, France.

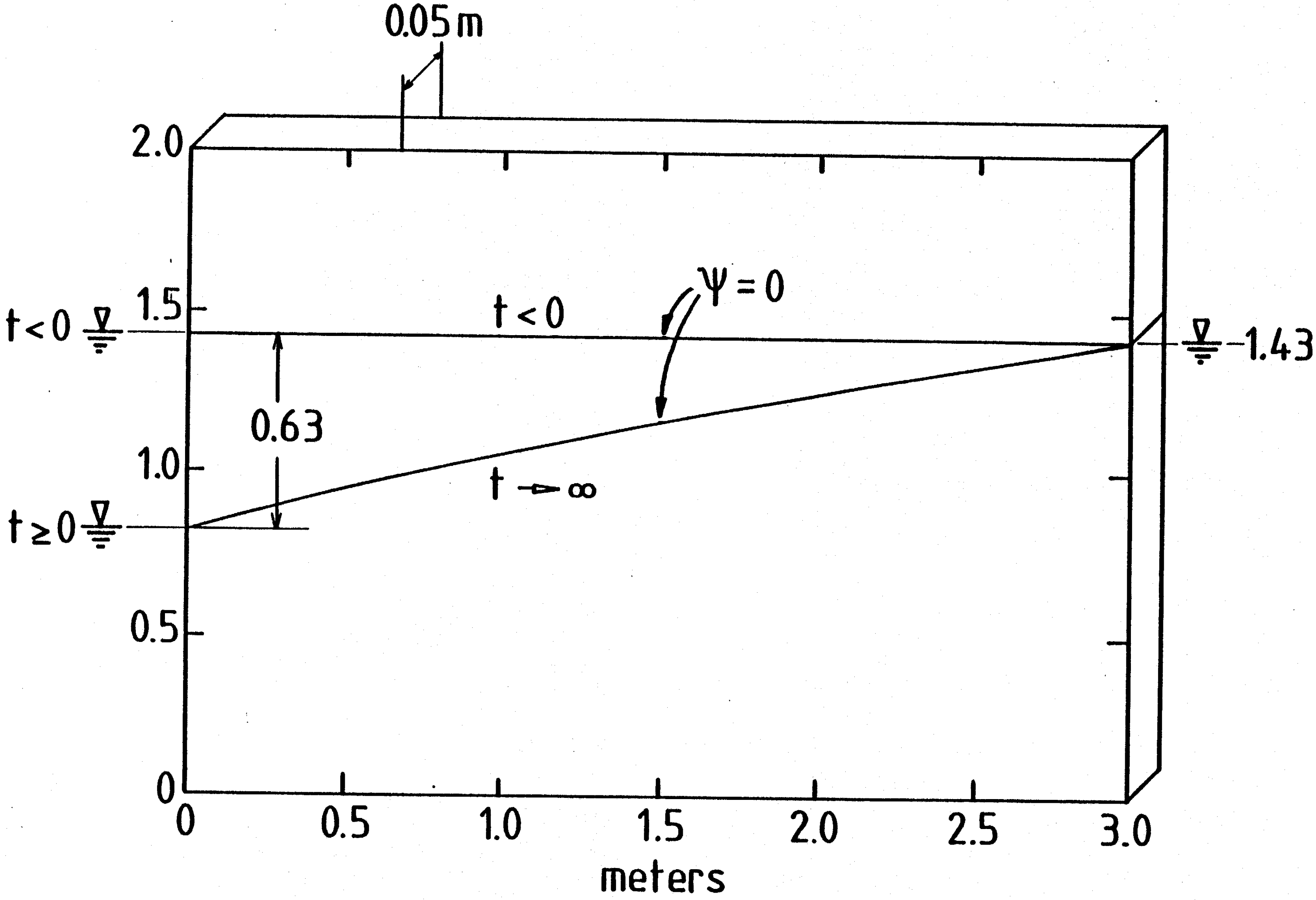
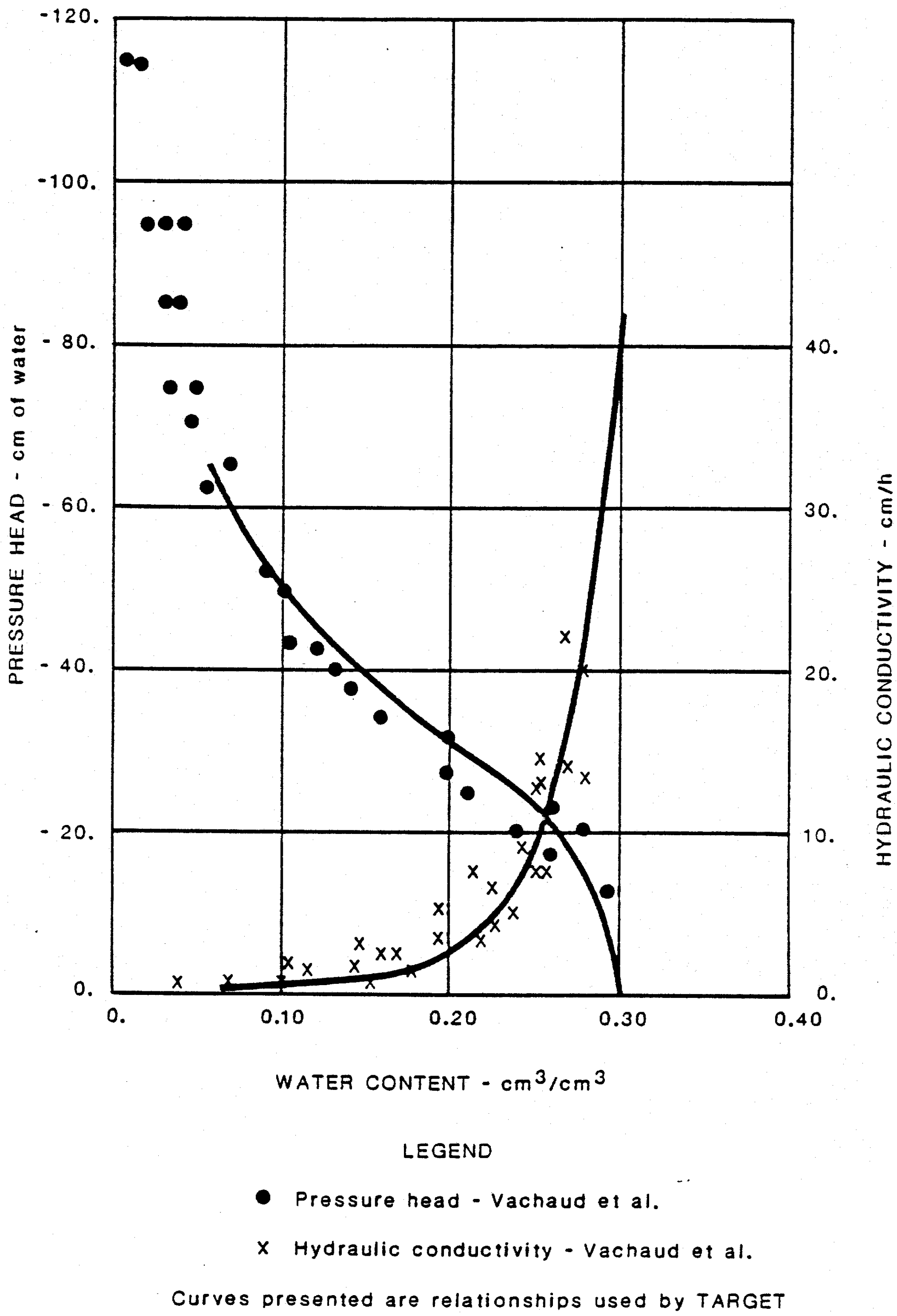


Figure 4-1
Schematic Diagram
Falling Water Table Simulation



Hydraulic Conductivity – Water Content – Water Pressure Head Relationships Comparison of TARGET Model Simulation vs Experimentally Obtained Data

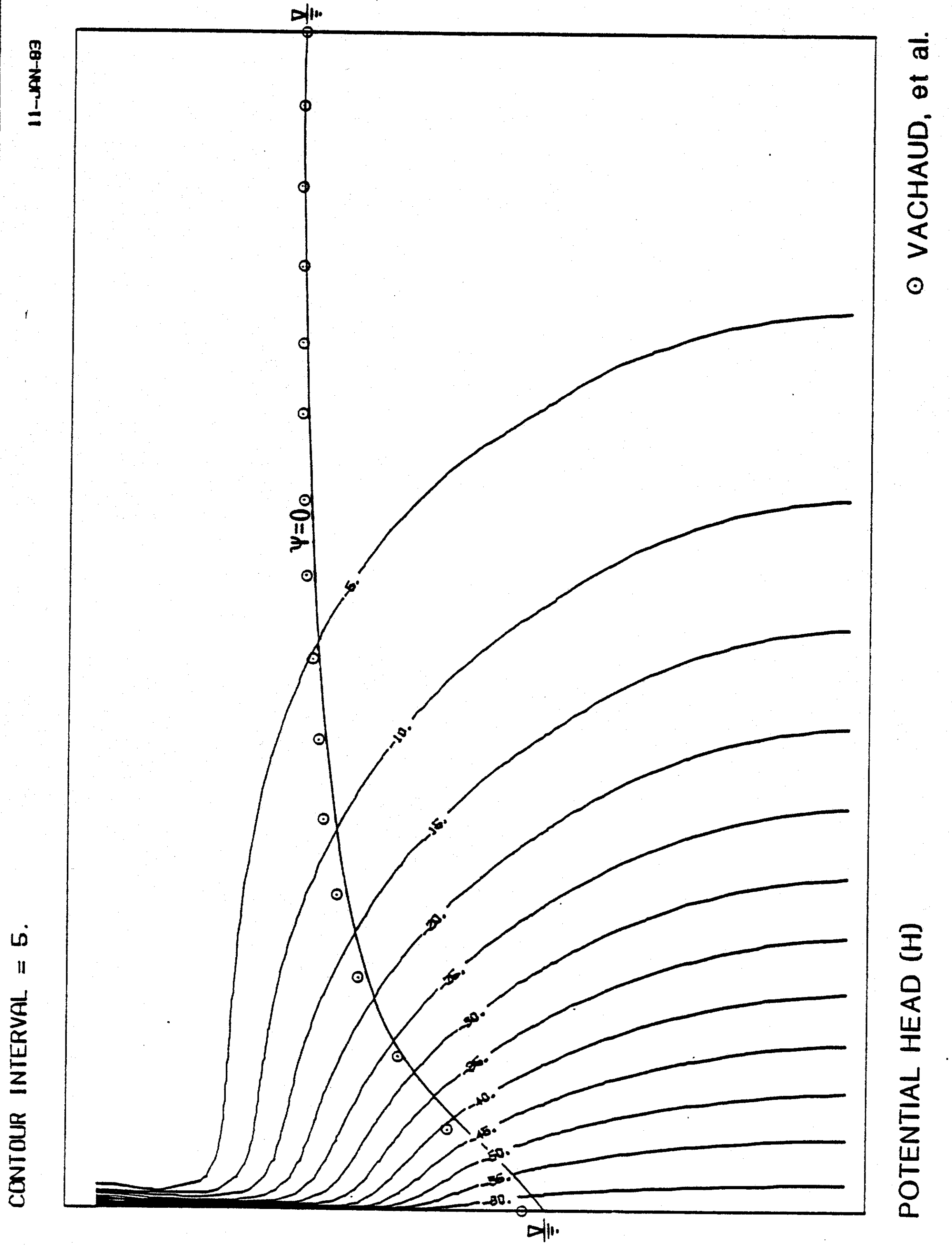
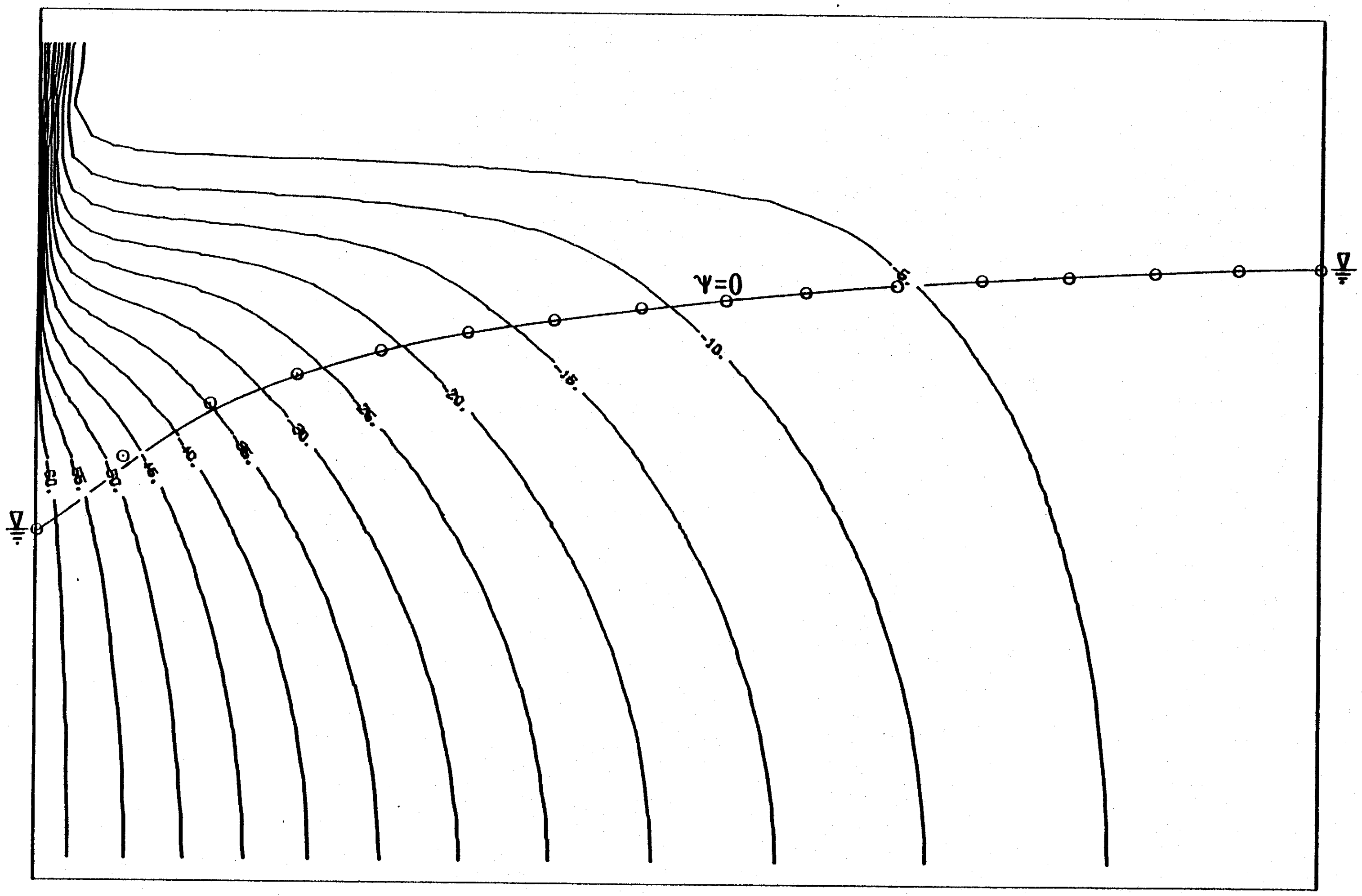


Figure 4-3
Plot at Time = 108 Step = 17

CONTOUR INTERVAL = 5.

11-JAN-83



POTENTIAL HEAD (H)

⊙ VACHAUD, et al.

Figure 4-4
Plot at Time = 360 Step = 31

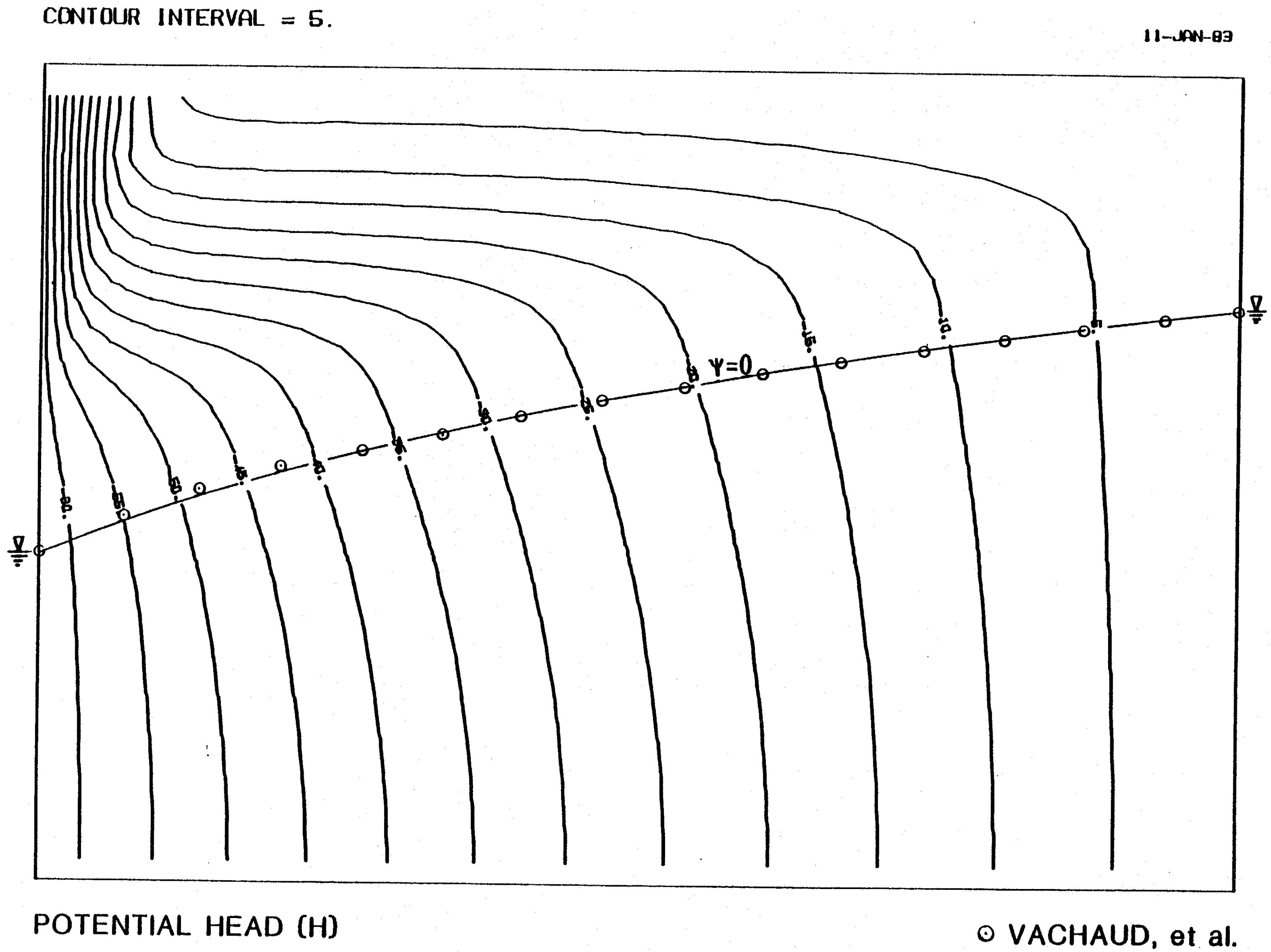


Figure 4-5
Plot at Time = 3,600 Step = 73

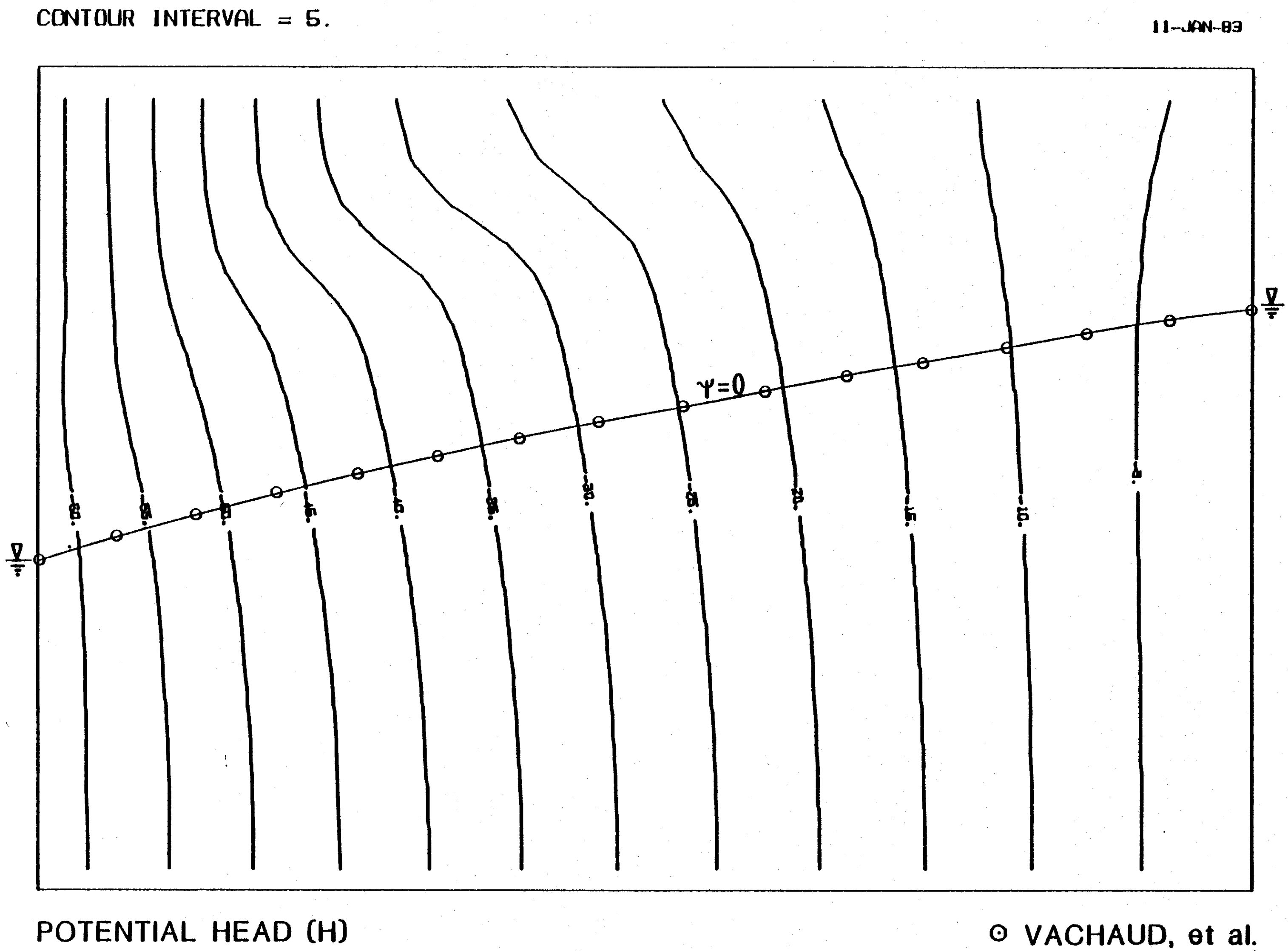


Figure 4-6
Plot at Time = 36,000 Step = 129

CASE 7: TARGET_2DH VALIDATION - COMPARISON TO USGS MODEL

Mine Pit Backfilling Investigation
Generated March 1983

Objective: This validation case resulted from an actual Dames & Moore project. The model was used to predict the hydraulic head distribution in the area of the Jackpile-Paguate Uranium Mine in New Mexico before and after mining activities. The results were used to recommend the degree of backfilling necessary to reclaim the mined area. It was desired to restore the water table to conditions similar to its original, natural state. The long-range effects of the backfilling efforts on water table recovery were predicted.

Following Dames & Moore's modeling using the TARGET model, the USGS also modeled the problem. They used their generic, two-dimensional ground-water flow model. The results of these two modeling efforts are presented in this case.

Description: The Jackpile-Paguate Mine is comprised of three major open pits and a major underground mine. The mine is located in an area of rough and broken terrain ranging in elevation from 5700 to 7000 feet. The topographic features are characterized by broad mesas and plateaus interspersed with deep canyons, dry washes, and broad valleys. Two major surface streams flow in the vicinity of the mine. As part of the proposed reclamation plan, open pit mines are to be backfilled to an elevation 3 feet above the anticipated post-reclamation water table recovery elevation. Modeling was used to estimate the maximum probable recovery elevation of the water table in the pits.

Little pre-mining ground-water data were available for the area. Estimated pre-mining contours of ground-water elevation were also developed for the project using the TARGET model. Except locally near open pits and outcrops, ground water in the area is confined.

Specification: The input parameters supplied to the model by Dames & Moore are presented below. These parameters were used also by the USGS to the extent possible in order to maximize the similarity of modeled conditions.

The finite difference grid used consisted of 42 cells in the east-west direction and 34 cells in the north south direction. The cell sizes ranged from 500 feet by 500 feet to 6000 feet by 8000 feet. The smaller cells were concentrated in the area of the mine pits.

The upper boundary of the model, the left boundary, and the right boundary all were set as zero flux (impermeable) boundaries. In order to simulate the outcrop of the Jackpile Sandstone and its contact with alluvium along the Rio Paguate and Rio Moquino (the two major streams), an area of high hydraulic conductivity was placed along the lower portion of the grid and a fixed head was placed along the lower edge of the grid. A fixed head was also placed at the upper reach of the Rio Paguate alluvium to allow simulation of the interconnection of the Rio Paguate and the Rio Moquino surface streams along the extent of the alluvium. The fixed head was set at an appropriate elevation in two nodes to simulate ground-water levels in alluvium along the Rio Paguate and its uppermost interconnection with the Jackpile Sandstone. By fixing the heads in these nodes, ground-water levels in nodes representing alluvium downgradient closely approximate those encountered in the field. Recharge to the system was simulated by a constant flux over a large areal portion of the aquifer. This combination of boundary conditions allows simulation of ground-water flow from recharge areas to outcrop areas.

The thickness of the Jackpile Sandstone was input to the model on a cell-by-cell basis based upon a detailed map showing thickness of the unit at several hundred drill hole sites. The combination of saturated thickness and hydraulic conductivity of the Jackpile Sandstone was used in the model to estimate transmissivity on a cell-by-cell basis.

The hydraulic conductivity varied from cell to cell in the model based on actual conditions. The values supplied to the model varied from 0.05 to 22 ft/day except for backfill material which was modeled as 190 ft/day.

The storage coefficient for confined conditions in the Jackpile Sandstone was modeled based upon a specific storage of 2.5×10^{-6} ft^{-1} and the local thickness of the aquifer. For unconfined conditions, a storage coefficient (specific yield) of 0.20 was used in the model. Total porosity of the Jackpile Sandstone was estimated at about 28 percent based upon an in-situ density of 120 pounds per cubic foot.

Total porosity of backfill was estimated at 45 percent. The initial volumetric moisture content was measured at approximately 15 percent. Therefore, an unconfined storage coefficient of 0.30 was utilized in the model. The backfill is never under confined conditions and, therefore, a confined storage coefficient is not required for the backfill material. Virtually no changes occur in water levels in alluvium, therefore, the model is insensitive to the values chosen for storativity of the alluvium.

Recharge to the aquifer was estimated to range between 0.12 to 0.24 in/yr. The total recharge rate to the model was 12,700 ft^3/day (66 gpm).

In order for the USGS to perform modeling comparable to that of Dames & Moore, two modifications to the USGS model were incorporated since the numerical solutions employed by the two models are different. First, the TARGET model requires that all cells (including the perimeter boundary) have a finite transmissivity. The USGS model was modified to match the TARGET model's requirement of a minimum transmissivity based on an equivalent thickness of 0.10 foot of saturated aquifer.

The second modification concerns the treatment of the modeled outcrop boundary. The TARGET model's requirement that cells have a finite transmissivity causes a small, steady ground-water flow through outcrop areas. This treatment was abandoned in the USGS model to allow cells to completely desaturate. This change allowed a steady-state simulation to be completed and further improved the agreement between the models for the simulated pre-mining steady-state hydraulic-head distribution.

The USGS modeling effort also varied from the Dames & Moore effort in its simulation of field conditions in the model. The larger cells in the finite-difference grid were split into two cells in order to increase numerical stability in the USGS model.

Results: The results of the model comparisons are presented in Figures 7-1 through 7-9. Three scenarios are represented in these figures, and are labeled as follows:

Case 1 - Pre-mining simulation
Case 2 - Post-mining simulation
Case 3.5 - Post-mining simulation with recommended in-pit dam installed

The figures present comparisons over the entire modeled area, the immediate mine area, and also presents cross sections along selected grid rows through the mine area. The following is a list of these figures.

Figure 7-1 Case 1, entire area
Figure 7-2 Case 3, entire area
Figure 7-3 Case 1, detailed area
Figure 7-4 Case 3, detailed area
Figure 7-5 Case 3.5, detailed area
Figure 7-6 Case 3.5, cross section, entire area, D&M row 14
Figure 7-7 Case 3.5 cross section, entire area, D&M row 21
Figure 7-8 Case 3.5 cross section, detailed area, D&M row 14
Figure 7-9 Case 3.5 cross seciton, detailed area, D&M row 21

Discussion: As can be seen in the accompanying figures, the results of simulation of the mine pit backfilling presented herein are consistent. In the simulation of the pre-mining case, the results from the two models are generally within 5 feet in computed heads. For the post-mining simulations, the results also agree closely except in the vicinity of the outcrop of the aquifer, where the USGS model computes heads that are commonly more than

40 feet higher than the TARGET model. These discrepancies diminish rapidly with distance from the outcrop.

In performing the comparison, the USGS stated in the discussion of their report that they found "no inconsistencies of a mathematical or programming nature which significantly affected its results" when discussing the TARGET model.

References:

Dames & Moore, 1983. Evaluation of Hydrologic Effects Resulting from Pit Backfilling, The Anaconda Company's Jackpile-Paguate Uranium Mine, Valencia County, NM, Consultant Report dated March 23, 1983.

USGS, 1984. Results of Simulations Using a U.S. Geological Survey Generic Two-Dimensional Ground-Water-Flow Model to Process Input Data from the Dames & Moore Ground-Water-Flow Model of the Jackpile-Paguate Uranium Mine, New Mexico, USGS Report Transmitted August 23, 1984.

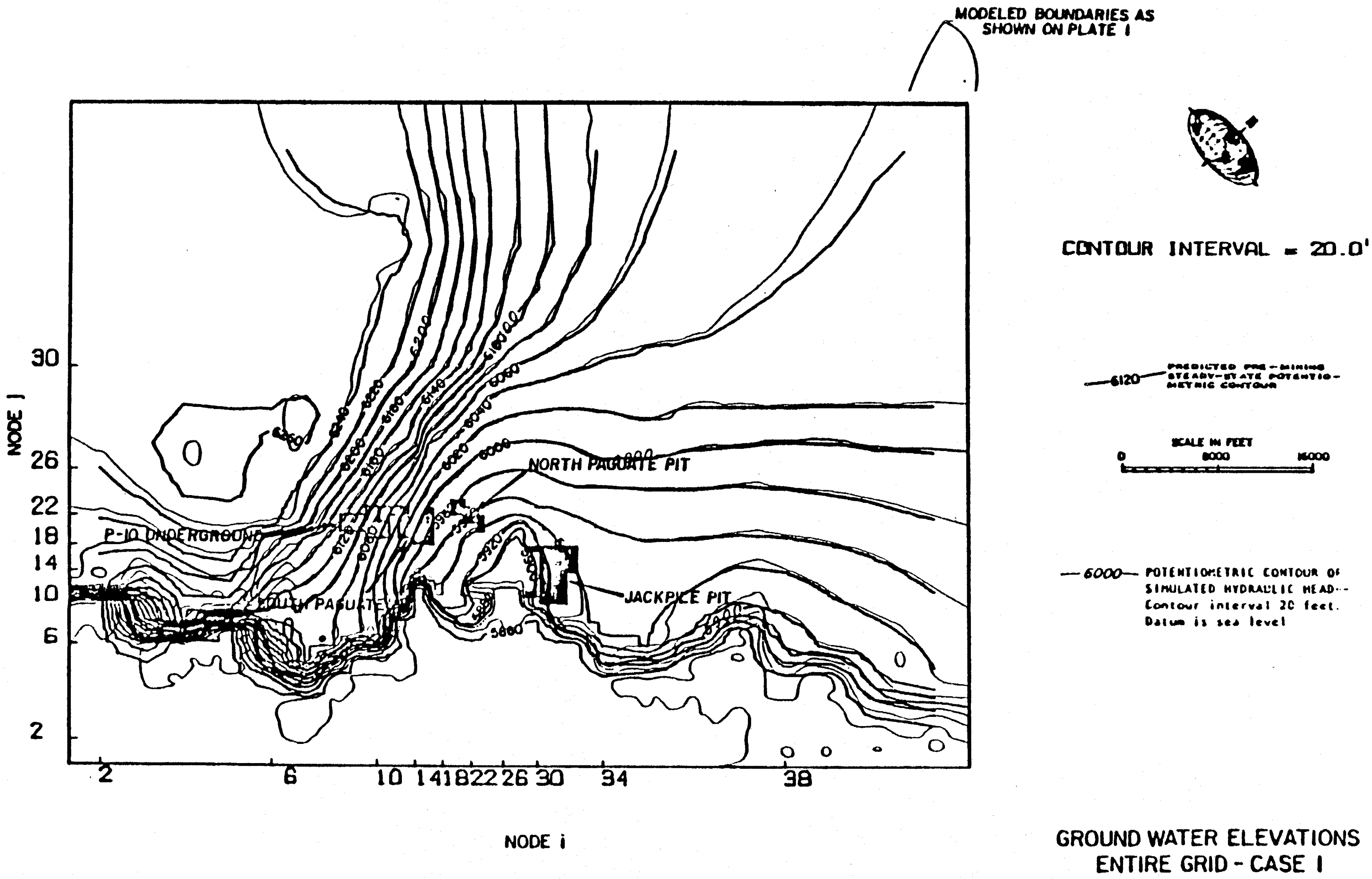


Figure 7-1. Map showing simulated pre-mining potentiometric heads in the entire modeled area for the simulation "decay780".

PLATE 9A

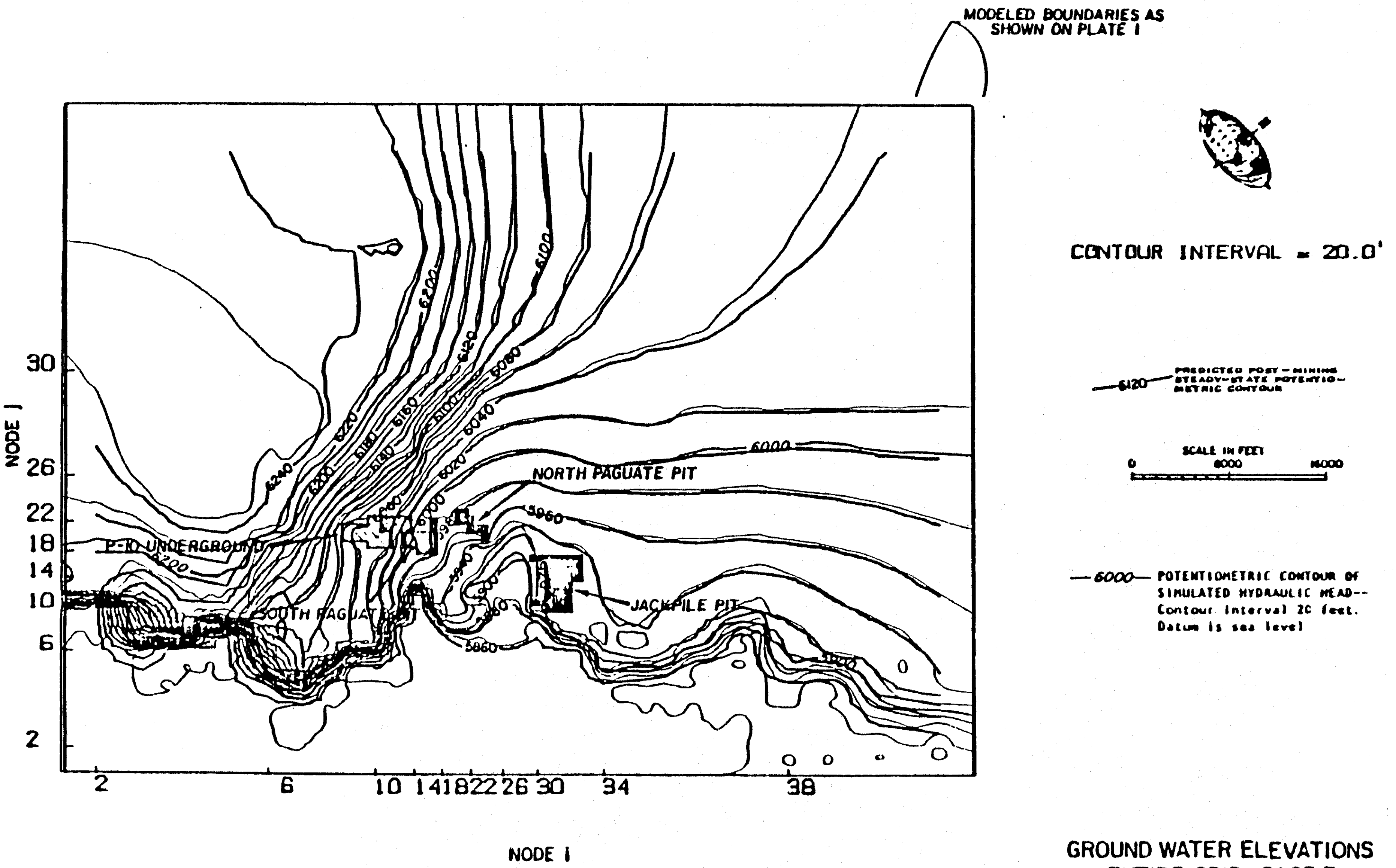


Figure 7-2. Map showing simulated post-mining and post-reclamation potentiometric heads (without artificial hydraulic barrier) in the entire modeled area for the simulation "case3".

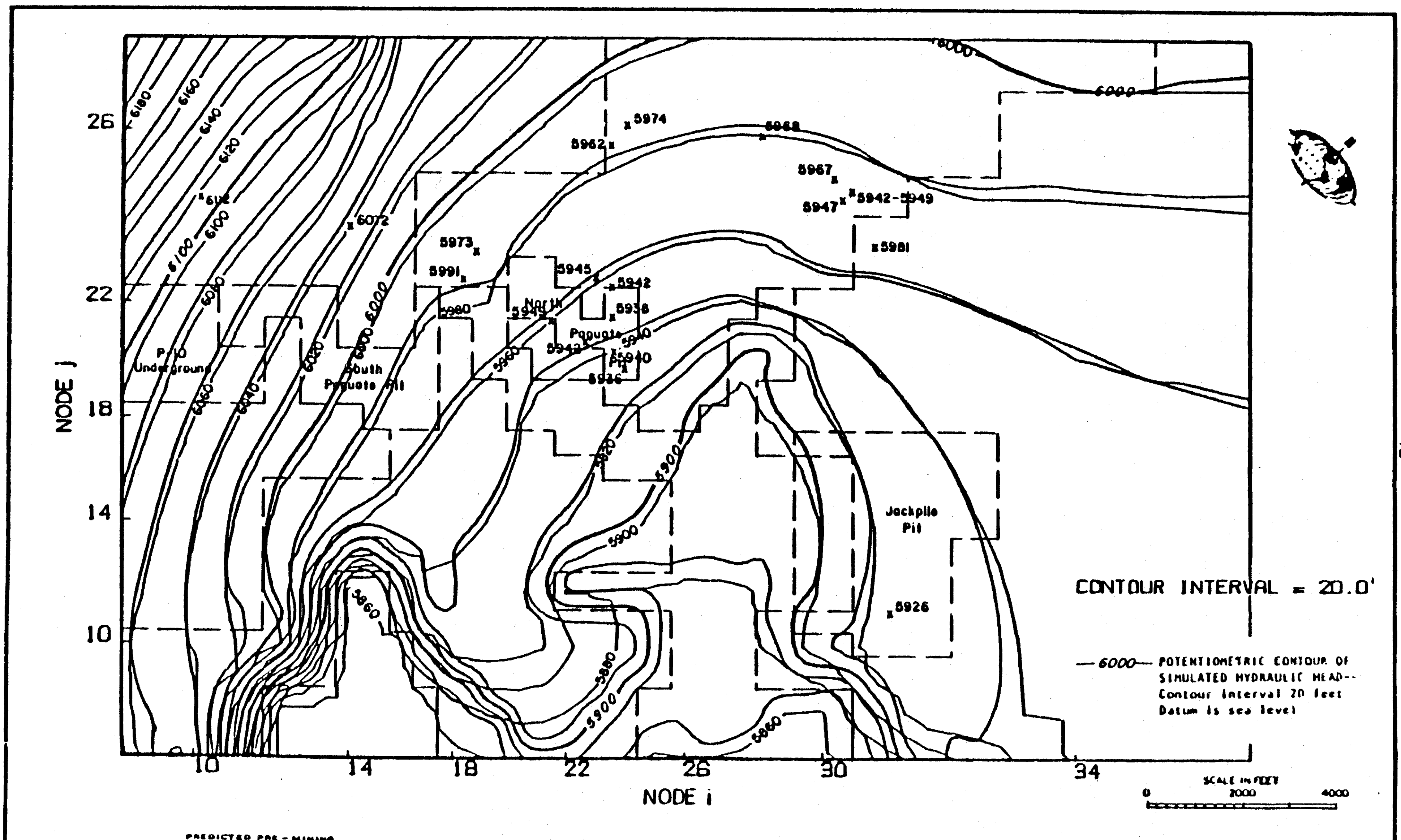
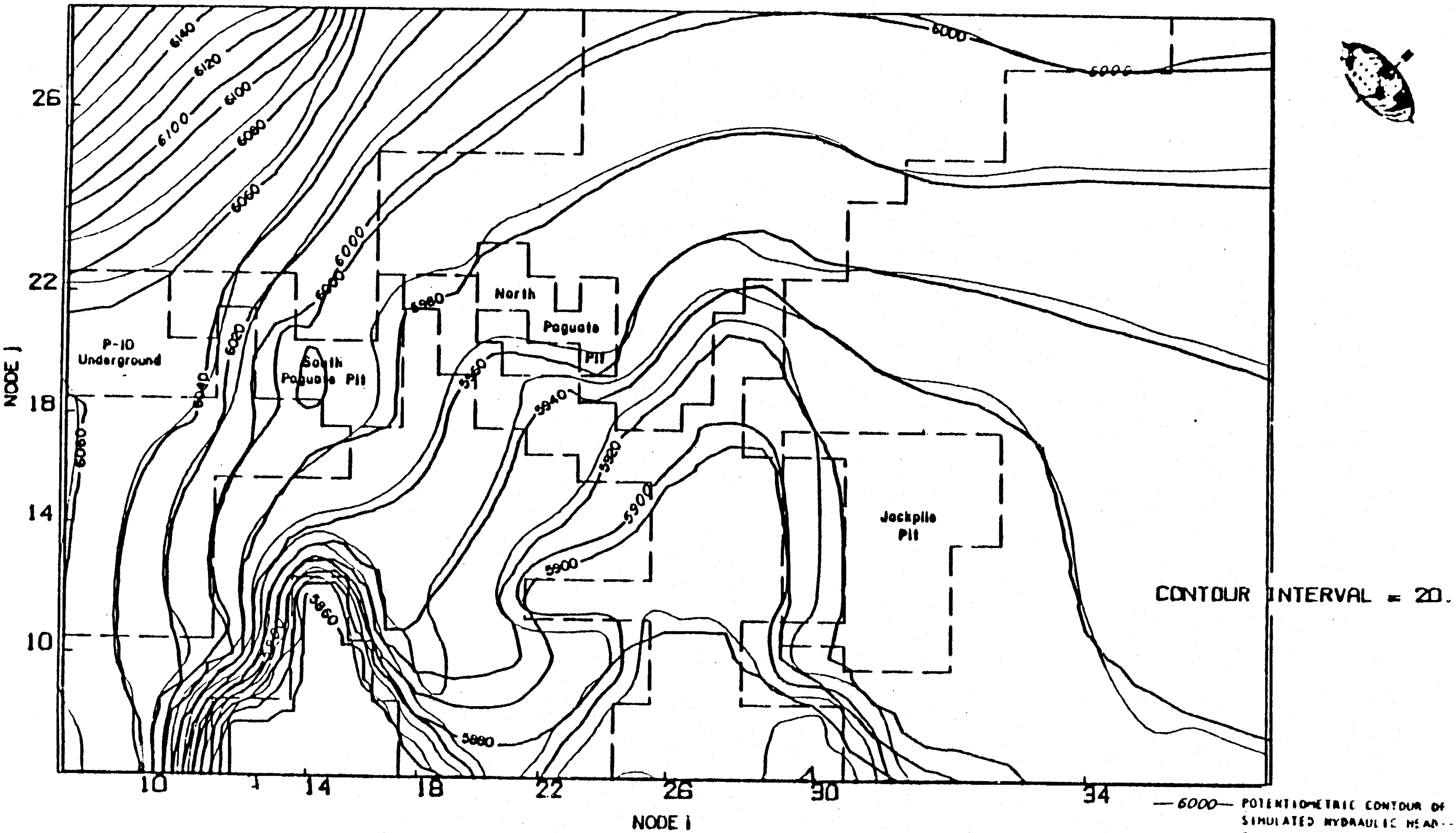


Figure 7-3. Detailed map showing simulated pre-mining potentiometric heads in the immediate mine area for the simulation "decay780".



—6120— PREDICTED POST-MINING STEADY-STATE POTENTIOMETRIC CONTOUR

SCALE IN FEET 0 2000 4000

—6000— POTENTIOMETRIC CONTOUR OF SIMULATED HYDRAULIC HEAD-- Contour interval 20 feet. Datum is sea level.

GROUND WATER ELEVATIONS
DETAILED AREA - CASE 3

Figure 7-4. Detailed map showing simulated post-mining and reclamation potentiometric heads (without artificial hydraulic barrier) in the immediate mine area for the simulation "case3".

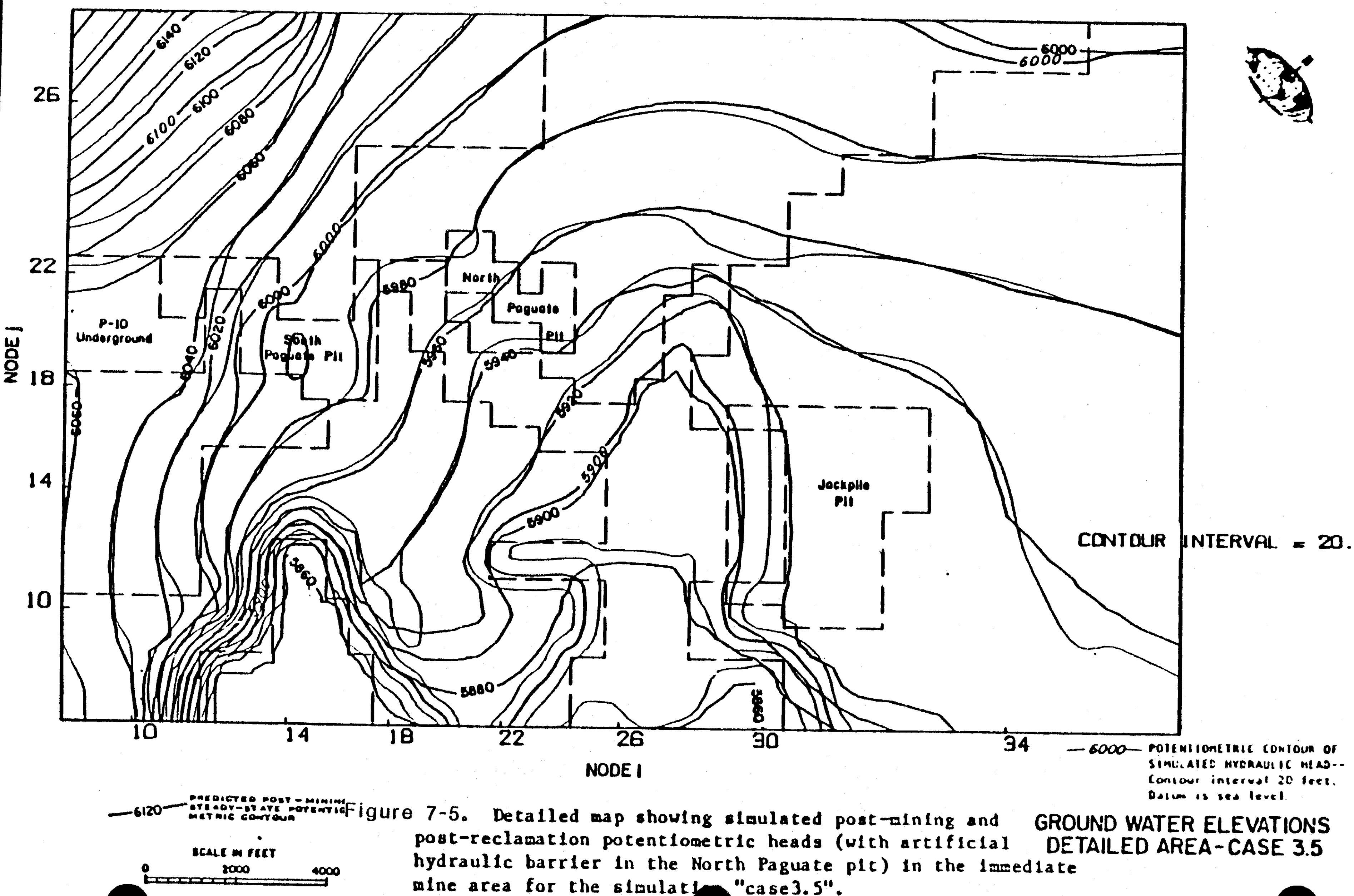


Figure 7-5. Detailed map showing simulated post-mining and post-reclamation potentiometric heads (with artificial hydraulic barrier in the North Paguate pit) in the immediate mine area for the simulati[illegible] "case3.5".

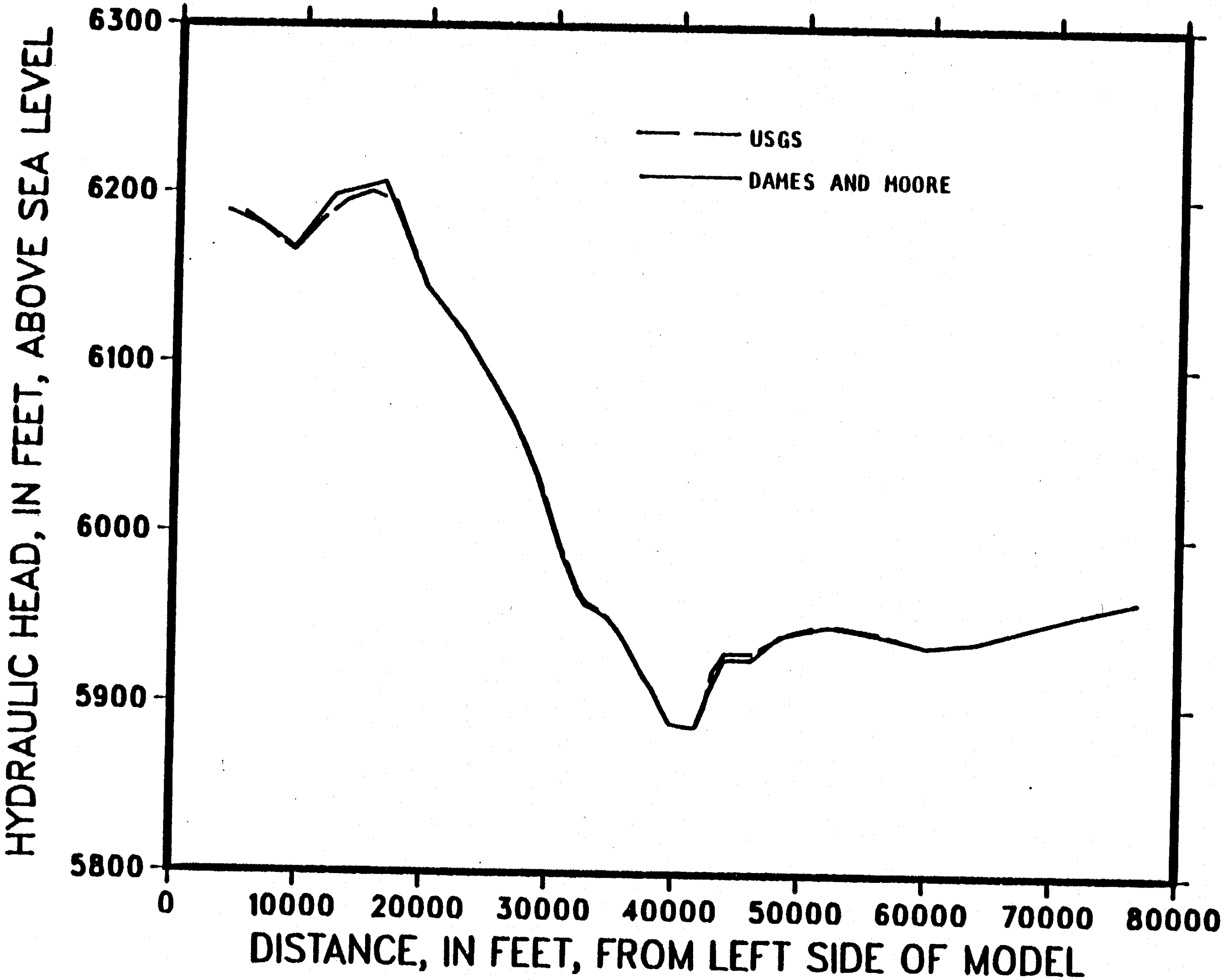


Figure 7-6. Cross-section of the entire modeled area along Dames and Moore model row 14 (USGS model row 28) through the Jackpile mine showing post-reclamation hydraulic heads for the simulation "case3.5".

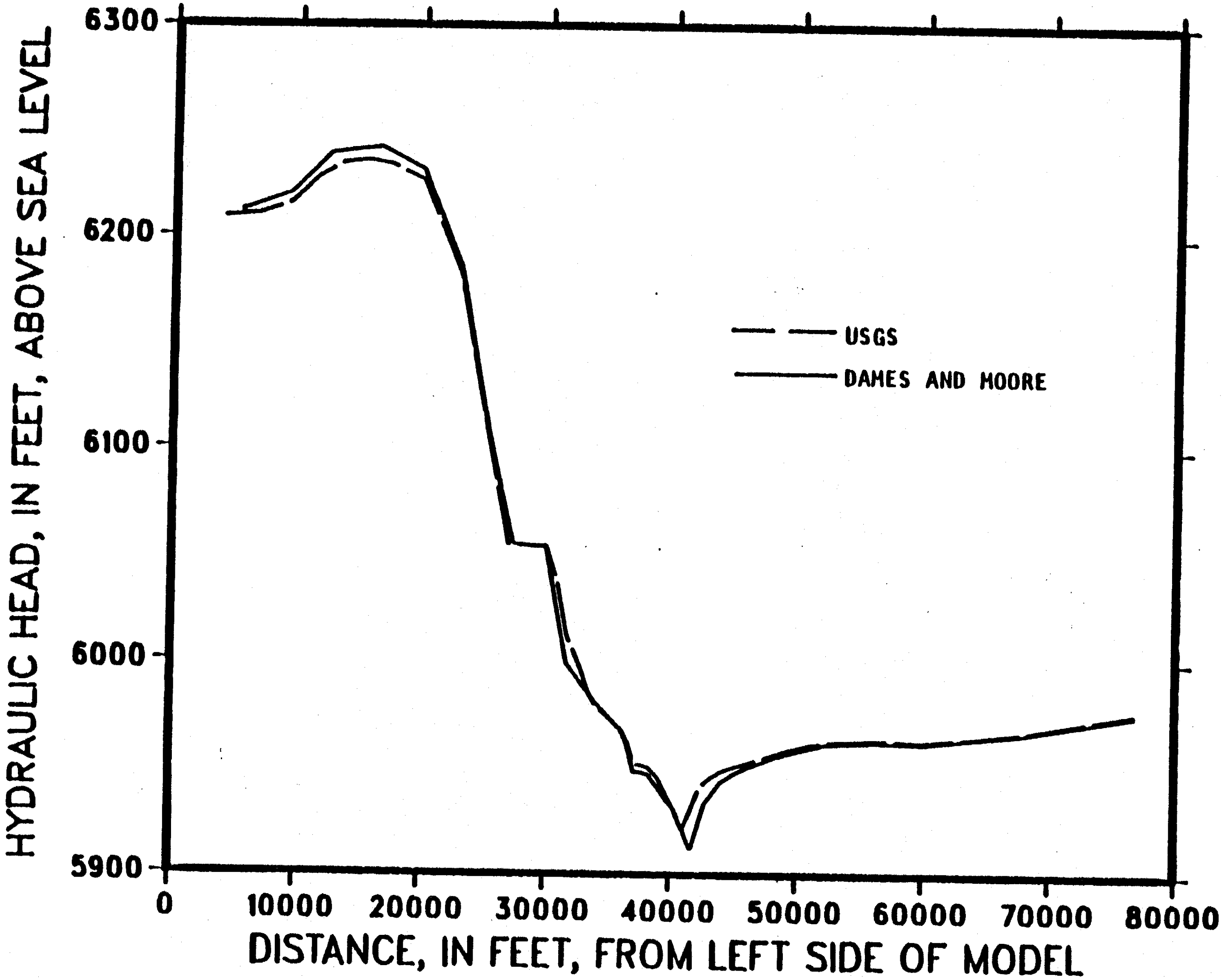


Figure 7-7. Cross-section of the entire modeled area along Dames and Moore model row 21 (also USGS model row 21) through underground mine P10, South and North Paguate mines showing post-reclamation hydraulic hea[illegible] for the simulation "case3.5".

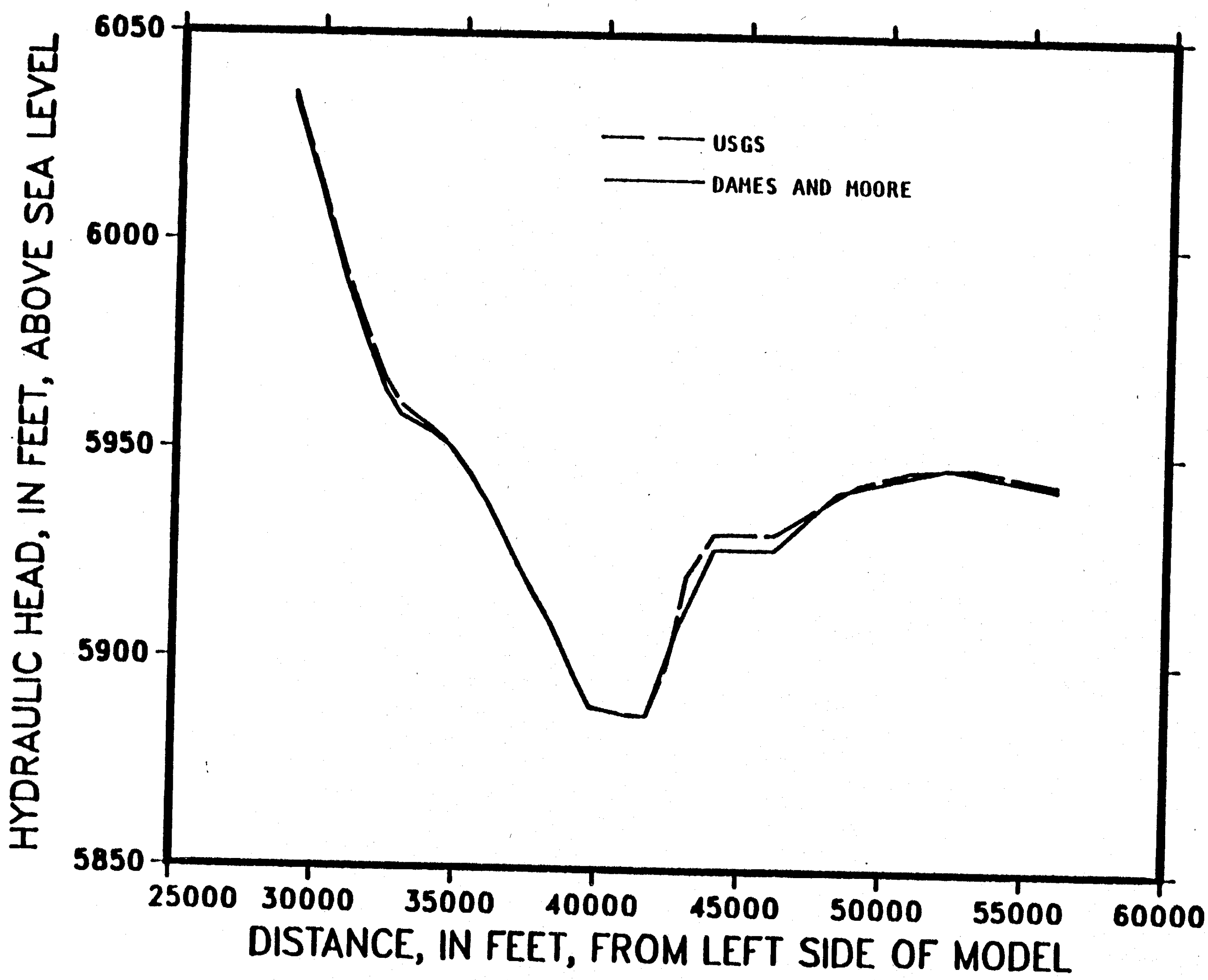


Figure 7-8. Cross-section of the detailed area of the model along Dames and Moore model row 14 (USGS model row 28) through the Jackpile mine showing post-reclamation hydraulic heads for the simulation "case3.5".

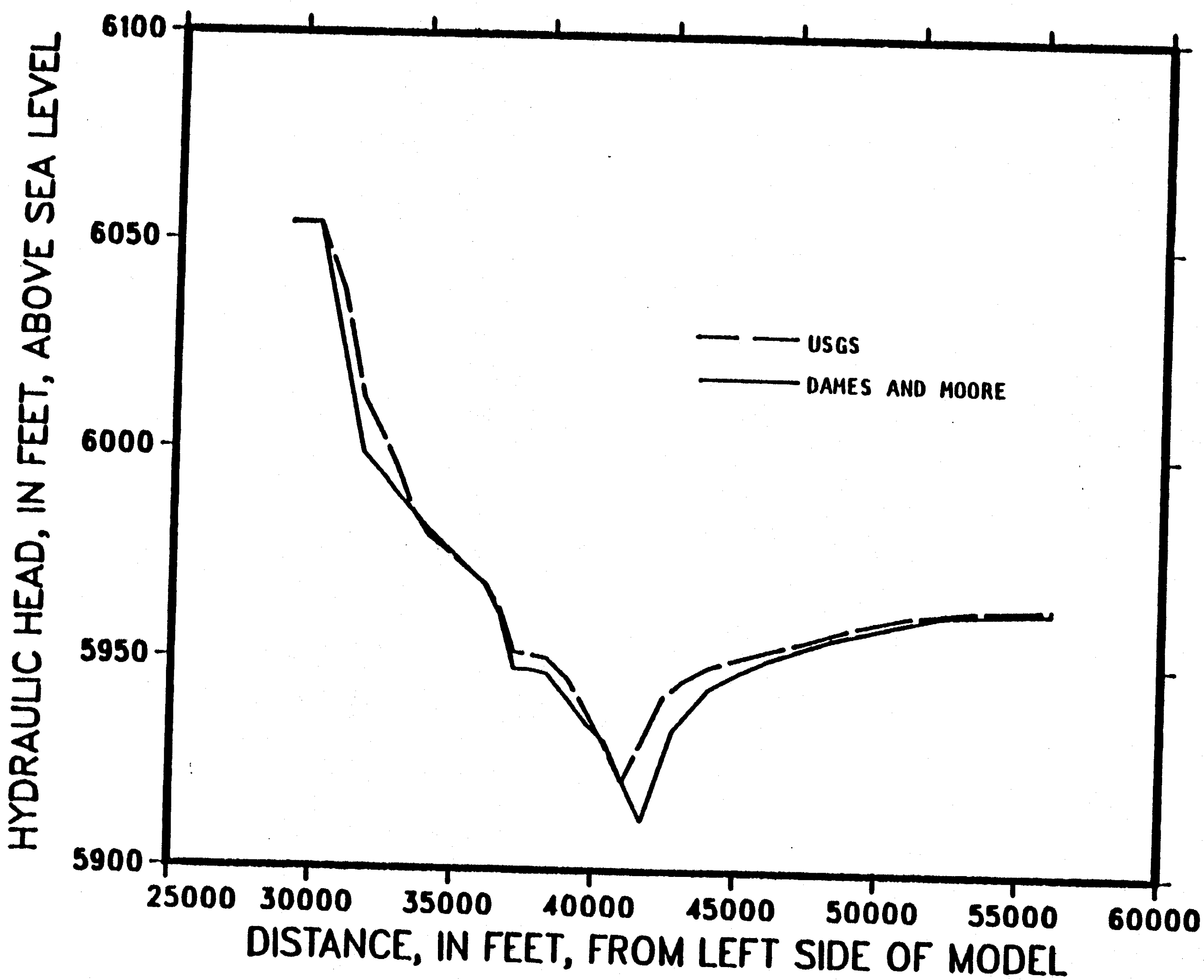


Figure 7-9. Cross-section of the detailed area of the model along Dames and Moore model row 21 (also USGS model row 21) through underground mine P10, South [illegible]d North Paguate mines showing post-reclamation hydraulic [illegible]s for the simulation "case3.5".

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SUMMARY OF
GROUND-WATER MODEL (TARGET) REVIEWS

The purpose of this document is to summarize peer, federal agency and state agency reviews of the TARGET model with a view to clarifying the context and outcome of significant reviews. The objective of most of the reviews documented here was to establish validity of the model/assumptions/data for the site in question. Quite frequently the reviews were undertaken with ensuing public review or litigation in mind. Dames & Moore testing and validation of the TARGET models is described in the model documentation and not considered here.

Attachment 1 provides a list of projects in which ground-water modeling formed a significant portion of the study and elicited separate review. A range of different agencies have been involved, in at least one case an external expert was involved in assisting agency review. In some of the cases listed here additional model calculations were requested to cover a wider range of site conditions, but at no time have the basic tenets of the model remained under question.

Two of the model reviews listed in Attachment 1 are described further in Attachment 2 and 3 (the original letters and reviews excerpted in Attachments 2, 3 and 4 are available for review on request). Attachment 2 contains the text of a letter from the U.S. Geological Survey (USGS) to the Bureau of Land and Minerals Management concerning verification of model predictions for the Anaconda Minerals Jackpile-Paguate Mine, New Mexico. The conclusions of the USGS study "established that the model used by Dames & Moore contained no inconsistencies of a mathematical or programming nature which significantly affected its results".

Attachment 3 covers an EPA review of model documentation, users guides, validation cases and 3D source listing prior to model application at a Superfund site in Baton Rouge, Louisiana. Review of the technical approach proposed at this site was particularly sensitive due to on-going litigation. The conclusions of the review state that "the theory and logic presented appear to be suitable to perform reasonably reliable simulations". In addition, it was recommended that the EPA rely on the TARGET code at the site under question, with the proviso of a comprehensive sampling and monitoring plan.

Attachment 4 consists of the general review comments on the TARGET package provided by Professor Allan Freeze. This review was solicited by Dames & Moore in the interests of refining the model documentation prior to sale of the TARGET models. Freeze's general comments indicate that "the TARGET package is versatile and powerful" while noting that the level of sophistication in the Physical and Mathematical Background chapter may be beyond typical engineers in small consulting firms. The specific comments elaborate on the general comments with reference to portions of the documentation, and have not been reproduced here.

The reviews described here, in combination with model documentation and validation as well as publication of theory and predicted results, provide the basis for background substantiation of model predictions.

ATTACHMENT 1

List of Projects in Which TARGET Predictions Were Reviewed and Accepted by State and Federal Agencies

Client	Date	Version of TARGET	Agency	Notes On Project Status
Amoco, Salt Lake City	5/85	2DU/2DH	EPA, State of Utah	Project Complete, Permit Pending
Anaconda Blue Water	3/81	2DU	NMEID	Project On Hold
Anaconda Minerals	2/84	2DU	USGS, BLM	Modeling Approved, EIS Being Finalized
Chem-Security	7/84	2DU/2DH	EPA	Modeling Complete
Chevron, Salt Lake City	3/85	2DU	EPA, State of Utah	ACL Petition
Federal American Partners	12/80	1DU/2DU/2DH	Wyoming DEQ	Project On Hold
Motorola, Phoenix	12/83	2DH/2DU/3DS/3DU	ADHS, ADWR, EPA	Continuing
Olean/NYSDEC	3/85	3DS	EPA, NYSDH	RI/FS Being Finalized
Petroprocessors, Inc.	6/85	2DU/2DH	EPA (Washington)	Pre-Project Model Approval Was Required
Phelps-Dodge	5/84	2DU/2DH	NMEID	Permit Approved
UMTRAP	82 & 83	2DU	DOE	Status Unknown
Gulf + Western	10/85	2DU	Colorado DOH, EPA	Continuing
Waste Management, Inc.	11/85	2DU	EPA (Ohio)	Model Approved, Project Continuing
Kentucky Avenue/ NYSDEC	11/85	2DH	EPA, NYSDH	Continuing

USER REFERENCES

This section provides brief descriptions of several projects, with references, in which the model and its application came under close scrutiny by the client and/or state or federal agencies or which involved sale of the models discussed in this proposal.

Project:	Remedial Investigation/Feasibility Study
Location:	Phoenix, Arizona
Owner/Client:	Motorola, Inc.
Reference:	Mr. Robert Lee, Motorola (602) 244-3911 Mr. Philip Briggs, Deputy Director, Arizona Dept. of Water Res. (602) 255-1586
Completion Date:	August 1986
Scope of Work:	Modeling was used at an early point in this project to aid in providing guidance and direction for determining the location and screened intervals of monitoring wells. It was recognized that TCE contaminants were occurring as a separate phase fluid and that contaminant movements were driven in part by density differences between the TCE and ground water. A fully three dimensional model accounting for density differences was used to perform sensitivity analyses to determine the influence of recharge, formation geometry and formation hydraulic conductivity. These studies indicated that detailed information on formation geometry was needed in the contaminant source areas. The model was subsequently used to understand the complex existing distribution of contaminants and the mechanisms of transport. This understanding allowed the approximate edges of the plume to be calculated with confirmational field monitoring rather than defining the edge of the plume through exhaustive field studies. The calibrated model will be used in the future to evaluate the effectiveness of alternate remedial action proposals.

Project:	Closure/Post Closure Plans - Remote Hazardous Waste Management Facilities
Location:	Salt Lake City, Utah
Owner/Client:	Amoco Oil Co.
Reference:	Mr. Dan Drumiler, Supt. Of Environmental Control & Safety, Amoco (801) 521-4831 Mr. Felix Flecas, Region VII, EPA (303) 293-1669
Completion Date:	May 1984
Scope of Work:	Modeling was used to predict the existing ground water flow paths and to analyze the effectiveness of selected closure options which included remedial action. Existing flow paths were predicted based on very limited data, to show that man-made canals acted as local hydrogeologic boundaries. Using the predictions, piezometers were drilled to provide field verification. The predictions were within 10% of the observed field values. Subsequently, the efficiency of collection ditches with slurry walls was evaluated as a function of collection ditch depth. The volume of flow to the ditches was calculated and a shallow ditch was found to be as effective as deeper ditches, at lower cost.

Project:	Alternate Concentration Limits Petition
Location:	Salt Lake City, Utah
Owner/Client:	Chevron USA, Inc.
Reference:	Mr. Mike Hannigan, Region 8, EPA (303) 293-1667
Completion Date:	March 1985
Scope of Work:	Modeling was used for several purposes to demonstrate the appropriateness of alternate concentration limits. It was used to accurately calculate the volume of ground water discharging to a receiving surface water canal. The ACL petition hinged, in part, on the dilution ratio of surface water to ground water flow rates. Modeling was also used to establish the maximum theore-

tical extent of contaminant transport under a variety of hypothetical situations including high rate pumping of an underlying aquifer, long term wet meterological conditions and long term dry meterological conditions.

Project:	Ground Water and Receptor Analysis Modeling
Location:	Baton Rouge, Louisiana
Owner/Client:	NPC Services Inc.
References:	Dr. Larry Bone, NPC Services Phone: (504) 292-6591 Mr. Peter Ornstein, Hydrogeologist, Office of Solid Waste and Emergency Response, EPA Phone: (202) 382-2063
Completion Date:	Model review complete, report review still underway.
Scope of Work:	Dames & Moore conducted ground-water mathematical modeling analyses at two sites to investigate the potential for contamination of multiple aquifers and to aid in design of a trigger monitoring network. Unusual site-specific features included seasonally-varying boundary conditions associated with the nearby Mississippi River.

Project:	Simulation of Recovery from Mine Dewatering
Location:	Jackpile-Paguate Uranium Mine, New Mexico
Owner/Client:	Anaconda Minerals, Inc.
Reference:	Mike Kernodle, Hydrologist, New Mexico District Office, U.S. Geological Survey Phone: (505) 766-1593 U.S.G.S Report "Results of Simulations using a U.S. Geological Survey generic two-dimensional groundwater flow model to process input data from the Dames & Moore groundwater flow model of the Jackpile-Paguate Uranium Mine, New Mexico," August 12, 1984.

Completion Date: August 1984

Scope of Work: The U.S. Bureau of Land Management, the U.S. Bureau of Indian Affairs, and the Pueblo of Laguna are in the process of assessing proposed reclamation measures for the Jackpile-Paguate uranium mine in west-central New Mexico. The operating company, Anaconda Minerals, retained Dames & Moore to model and project post-reclamation water levels in the pits. The simulations included pre-mining steady state analysis of flow in the Jackpile and Rio Paguate/Rio Moquino alluvial aquifers, analysis of post-reclamation water-level recovery within uniform backfill material, and analysis of water-level recovery with backfill material of variable properties. At the request of the Land and Minerals Management the U.S.G.S. undertook identical calculations with the Survey Model and found that the Dames & Moore model exhibited "no inconsistencies of a mathematical or programming nature which significantly affects its results."

Project: Hydrologic Investigations in Support of Groundwater Discharge Plan.

Location: Hidalgo County, Southwestern New Mexico

Owner/Client: Phelps-Dodge Corporation

References: Mr. Kent Bostick, Groundwater Hydrologist, State of New Mexico, Environmental Improvement Division
Phone: (505) 984-0020, Ext. 508

Completion Date: November 1983, August 1984

Scope of Work: Dames & Moore conducted, among other hydrologic investigations, predictions of the migration of contaminants from an evaporation pond in order to evaluate the effect of evaporation pond operation on water quality in the nearby Playas Lake. The lined but leaky evaporation pond is used to receive liquid effluent of high TDS from the smelter. A series of model simulations were used to:

- o Establish the depth to which contaminants are likely to migrate.

- Confirm estimated infiltration rates calculated on the basis of an approximate water balance.
- Calibrate uncertain model parameters through comparison of observed concentrations with those predicted.
- Predict the concentration levels which will occur in the vicinity of Playas Lake in the future.

The predicted extent and depth of contamination was corroborated by geophysical testing undertaken by the client.

Project:	Simulation of Chemical Seepage from Power Plant Solid Waste
Location:	Not applicable
Owner/Client:	Electric Research Institute/Acurex Corporation
Reference:	Dr. Larry Waterland, Program Manager, Acurex Corporation Phone: (415) 964-3200, Ext. 3618
Completion Date:	August 1981, February 1983, October 1984
Scope of Work:	The three projects involved mathematical modeling analyses of the migration of selected chemical species in the waste, through the liner (if present), in the unsaturated zone, and through the saturated aquifer beneath and adjacent to lined and unlined sludge landfills and ash ponds. In one instance ambient, long-term concentrations in a nearby river, resulting from the predicted pond overflow, were also analyzed. The overall purpose of the studies was to predict the likely concentrations of 13 chemical species in the groundwater, as a result of the 30-year operation of waste impoundments of various configurations, at two hypothetical drinking-water wells 1.0 and 2.5 km downgradient of facilities. The results of these studies were used in a risk evaluation of power plant integrated control configurations.

Project:	Technology Transfer (sale), TARGET 3D Ground Water Model
Location:	Phoenix, Arizona
Owner/Client:	Arizona Department of Water Resources
Reference:	Mr. Philip Briggs, Deputy Director, ADWR (602) 255-1586
Completion Date:	August 1986
Scope of Work:	Installation of codes and plotting programs on client's computer and 3 day training seminar for ADWR project mangers and staff in code use. ADWR is planning on using the codes for the evaluation of TCE movements at 2 superfund sites.

Project:	Technology Transfer, TARGET Ground-Water Models
Location:	Tokyo, Japan
Owner/Client:	Chiyoda Chemical Engineering Company
Reference:	Mr. Yanagawa, Chiyoda Dames & Moore Phone: 81-3-454-4741
Completion Date:	Installation complete, training yet to be undertaken.
Scope of Work:	Transfer of the five models involved the following tasks:

1. Delivery of five TARGET codes and documentation.
2. Assistance with conversion of codes from VAX versions to IBM versions.
3. Training seminar.

Project:	Transfer of three TARGET models
Location:	Horsham, England
Owner/Client:	Electrowatt Engineering Services (UK) Ltd.
Reference:	Mr. Stephen D. Lympany Phone: 44-1-403-50131
Completion Date:	July 1985
Scope of Work:	Delivery of three TARGET codes and documentation.

ATTACHMENT 2

Memorandum From

United States Department of Interior

Geological Survey, Reston, VA 22092

(Text of Letter Reproduced In Full Below)

August 23, 1984

Memorandum

To: Assistant Secretary -- Land and Minerals Management

Through: Assistant Secretary -- Water and Science

From: Director, Geological Survey

Subject: PUBLICATIONS- Report "Results of simulations using a U.S. Geological Survey generic two-dimensional ground-water-flow model to process input data from the Dames & Moore ground-water-flow model of the Jackpile-Paguate Uranium Mine, New Mexico"

In accordance with the agreement reached at the meeting of May 29, 1984, between yourself, Bureau of Land Management (BLM) Assistant Director Sokoloski, other representatives of BLM, and Philip Cohen, Gordon Bennett, and Roger Wolff of the Water Resource Division, U.S. Geological Survey (USGS), we are pleased to provide the accompanying two copies of the subject report.

In the work summarized in this report, USGS hydrologists of the New Mexico District office carried out a number of numerical simulations of the ground-water-flow system in the vicinity of the Jackpile mine. The simulations were performed using a standard USGS generic model for two-dimensional ground-water flow; they employed hydrologic parameters which in some cases were identical to those used in an analysis by Dames & Moore, Inc., and in some cases were systematically varied from those values.

In all, 14 simulations were carried out by USGS hydrologists. Initially, four simulations were run corresponding to Case 1 of the Dames & Moore analysis, which addressed the pre-mining steady-state condition of the aquifer. These four simulations differed from one another in the subdivision of the model mesh, in the way a particular aquifer outcrop was simulated, and in the way two streams, the Rio Paguate and Rio Moquino, were simulated; the hydraulic conductivity and recharge values used in all four of these simulations were identical to those used by Dames & Moore. Next, two simulations were carried out corresponding to Case 3 of the Dames & Moore analysis, which addressed the final post-reclamation condition, subject to the assumption that no low-permeability barrier would be emplaced in the North Paguate pit during reclamation.

These two simulations differed from one another only in the way the Rio Paguate and Rio Moquino were represented; the hydraulic conductivity and recharge values were identical to those of Dames & Moore. Finally, eight simulations were carried out corresponding to Case 3.5 of the Dames & Moore analysis, which again addressed the final post-reclamation condition, but with the assumption that a low-permeability barrier would be emplaced in the North Paguate pit during reclamation. Within this group, the first two simulations differed from each other in the way the streams were represented, but again, the hydraulic conductivity and recharge values used by Dames & Moore were retained. The final six simulations of this group, on the other hand, in-corporated various combinations of recharge and hydraulic conductivity which differed from those used by Dames & Moore. The variation in recharge consisted of an increase from 0.12 inches to 0.24 inches per year over a relatively small fraction of the modeled area. The changes in hydraulic conductivity involved uniform halving and doubling of the aquifer conductivity, and uniform halving and doubling of the conductivity of the backfill material in the reclaimed mine pits.

The USGS work established that the model used by Dames & Moore contained no inconsistencies of a mathematical or programming nature which significantly affected its results. The analysis further demonstrated that the changes in the method of simulating the outcrop and the streams produced significant water level differences only in the immediate vicinity of those features. Variation in recharge and hydraulic conductivity, on the other hand, caused significant water level differences within the reclaimed mine pits. In one simulation, in which the hydraulic conductivities of the aquifer and the backfill were doubled while the recharge values used by Dames & Moore were unchanged, the USGS results indicated lower post-reclamation ground-water levels in the Jackpile and South Paguate pits, but higher levels in the North Paguate pit. In the five other simulations in which parameters were varied, the USGS results indicated final ground water levels in the reclaimed pits that were higher by at least 20 feet, and commonly by as much as 50 feet, than those computed by Dames & Moore. These results illustrate the sensitivity of computed water levels to the assumed parameters, but do not in any way either corroborate or dispute the parameter values assumed by Dames & Moore. We point out again that to address this latter question a full hydrologic investigation, requiring at least 18 months' time, would be required.

ATTACHMENT 3

Memorandum From

United States Environmental Protection Agency

Washington, D.C. 20460

(Text of Covering Memorandum and Conclusions
Reproduced in Full Below)

May 17, 1985

MEMORANDUM

SUBJECT: Review of TARGET Code for use at Petro Processors Site

FROM: Peter M. Ornstein, Hydrogeologist
Physical Sciences Section, OWPE (WH-527)

THRU: Rob Clemens, Acting Chief
Physical Sciences Section, OWPE

TO: Tony Gardner
Region VI

Attached please find my review of Dames & Moore's TARGET computer code. Based on my review, I recommend that EPA accept the use of TARGET at the Petro Processors Site provided that a comprehensive monitoring and sampling plan is implemented. The plan should provide for monitoring contaminant levels in and around the predicted plume in the 40 foot zone to assist in code calibration and also provide for monitoring the 400 foot aquifer in selected locations to assure trigger level credibility.

In light of this recommendation, the Phase 2 review of TARGET does not seem appropriate. At such time as the agency has determined what peer review criteria and procedures will be employed for the selection and use of ground-water models, this and other model codes will, in all likelihood, be evaluated in greater detail on a generic basis.

Please call me at (FTS or 202) 382-2063 if you have any questions or comments.

CONCLUSION

As the purpose of this review is to recommend whether or not EPA may rely upon TARGET to produce reasonably reliable results at the Petro Processor's site, portions of the documentation not relevant to this purpose were not critically reviewed. In addition, any confidence in TARGET expressed herein must be qualified since the reviewer did not run the code and therefore did not have the opportunity to test or stress the code. Overall confidence in the TARGET code would be substantially improved if the code were in the public domain and used by others within the technical community.

In summary, TARGET employs a non-traditional approach to modeling contaminant transport in ground water by use of its guess and correct algorithm. Given the limited scope of this review, the theory and logic presented appear to be suitable to perform reasonably reliable simulations. No inherent deficiencies either in the guess and correct algorithm or in the way the hydrodynamics and mass transport have been treated are apparent.

It is recommended that EPA rely upon the TARGET code at the Petro Processor's Site. It cannot be overemphasized that use of TARGET must be performed in conjunction with a comprehensive sampling and monitoring plan. The monitoring and sampling is necessary to provide a "safety net" to counter the uncertainty associated with the site's complex hydrogeology as well as uncertainty associated with modeling the site (i.e., quality of data, applicability of generic assumptions to the site, etc.). Since the intended use of TARGET is to establish trigger levels in the 40 foot zone to protect the 400 foot aquifer, both zones should be monitored to enhance confidence in the predicted levels as well as aid in further field calibration and verification of the model.

To reiterate, the scope of this review focused on TARGET's use for a specific purpose at the Petro Processor's site. Until such time as the code has been peer reviewed and tested in the professional community and available in the public domain, evaluation of site by site applications is recommended.

ATTACHMENT 4

Letter From

R. Allan Freeze, Ph.D., P.Eng.

(Text of General Comments Reproduced
in Full Below)

July 10, 1985

Dr. D. A. Stephenson
Dames & Moore
3737 N. 7th Street, Suite 121
Phoenix, Arizona
U.S.A. 85014

Dear Dave:

In response to your letter of June 11, 1985, I reviewed the Dames & Moore TARGET package, giving special consideration to the suitability of the documentation for outside-the-firm release. I have divided my comments into general comments and specific comments.

GENERAL COMMENTS

1. It is clear to me that the TARGET package is a versatile and powerful set of computer programs for the mathematical modeling of groundwater flow and solute transport. The mathematical foundations are strong and the numerical methodology clever and efficient. It is clear that the authors of the program and the documentation are working from a strong technical base.

2. The writing style throughout the report is very clear. I will have some comments about the level and order of presentation, but I must emphasize that the current presentation of each topic, both in their descriptive and mathematical contexts, is very well done.

3. The major area of concern that I can identify lies in the level of sophistication in the chapter on the Physical and Mathematical Background of the models. This chapter uses a very sophisticated mathematical framework and a very advanced notation. As a research scientist in this field I find it compact and elegant, but my experience in dealing with small consulting firms who may provide a primary market for TARGET would lead me to question whether engineers from such firms would be at home with this level of presentation. One must ask to whom this chapter is directed. If it is directed to reviewers such as myself as a kind of base document that lays out the mathematical foundations of the programs for those few who may wish to follow it up, then the current presentation may be suitable. If, on the

other hand, it is intended as a kind of textbook to accompany training sessions for consulting engineers from smaller companies, then I believe it needs to be expanded and the order changed somewhat in order to bring it into line with the backgrounds that such "students" will have. Several of the Specific Comments pertain to this issue, but the more general suggestions are as follows:

(a) The Introduction should be expanded to include more complete descriptions of the types of boundary-value problems that the programs can handle (and the engineering problems to which they apply). It should include clear definitions of such concepts as steady-state and transient flow, unsaturated and saturated pressure heads, homogeneity and anisotrophy, etc.

(b) Section 2-0 on Physical Mechanisms and Chemical Processes should include detailed positive statements of the capabilities of the models with respect to groundwater flow and solute transport. In the current write-up the basic assumptions of Section 2-1-1 hit the reader without lead in or warning. Some of them are quite sophisticated and required a detailed understanding of the equations of groundwater flow. I would be inclined to save this list until after the primary development of Section 3-0.

(c) The references provided in the Introduction are a bit obscure. I would refer to the available textbooks by Wang and Anderson, Pinder and Gray, Remson et al, and to the AGU monograph by Bredehoeft et al and the NWWA monograph by Mercer and Faust.

(d) Much of the descriptive material is too terse. Two examples: (i) Section 2-2 on Solute Transport ought to summarize all the mechanisms of transport noting which ones are included and which ones are not; (ii) The discussion of seepage faces in the 2nd paragraph from the bottom of page 16 does not hint at the complexities associated with their simulation (iterative positioning of the exit point, problems associated with multiple seepage faces, etc.).

(e) There are many examples in the Specific Comment of cases where the readers first encounter with a concept or notation occurs in the midst of some other explanations. Examples: (i) on p. 26 just below Eqn. (4-38) the reader is first informed that the numerical solution is iterative; (ii) The Peclet number is introduced for the first time on page 3-1 in the Validation Chapter. In all cases, introductory material should have appeared earlier so that the reader is not taken by surprise.

(f) I would prefer to see variables defined at the point of first encounter as well as in the notation list. It is difficult for the reader to switch back and forth from the text to the list and to locate the particular symbol on the list.

4. In the Introduction it is stated that there are 5 models in the TARGET family, but there are 18 possible contaminations of the properties listed there. The 5 models should be identified clearly and examples of their use described. Model TARGET 2DH does not figure anywhere in the Background chapter or the User's Guides, but it appears in the first two validation cases.

5. The User's Guide to TARGET 2DU and TARGET 3DS are clearly done and should prove easy to follow by prospective clients. The Specific Comments note a few places where clarification is needed. I note, however, that a list clearly relating the computer acronyms to their mathematical notation in the Background chapter would be useful.

6. The chapter on the Summary of Validation Cases is clear and convincing. The only apparent capability of the TARGET family that is not fully validated is a case that involves solute transport in the unsaturated zone. If such a validation is available, it would make a worthwhile addition.